INVESTIGATION OF BIODEGRADATION PROCESSES IN SOLID WASTE LANDFILLS

THESIS

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Presented to the Faculty of the Graduate School of Engineering of the Air Force Institute of Technology

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In Partial Fulfillment of the Requirements for the

Degree of Master of Science in Engineering and Environmental Management

Philip A. Colborn, B.S.

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Philip A. Colborn

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Abstract

Greater demands on landfill capacity, stricter regulations intended to minimize landfill environmental impacts, and the economic potential associated with landfill operations have shifted the emphasis of landfill disposal toward methods concerned with the long-term performance and capacity of landfills. Two opposing philosophies have emerged in constructing and managing landfills: the "dry-tomb" and the "wet-cell." The key to managing a landfill from the wet-cell viewpoint is first understanding the biodegradation processes occurring within the landfill.

This thesis attempts to determine the fundamental processes responsible for the degradation of solid waste by employing a system dynamics approach. A system dynamics model is constructed that reproduces behavior of the landfill biochemical reactor system by identifying the biodegradation processes driving basic system behavior. The model utilizes landfill gas production as the measure of landfill behavior over time. The resultant model and model simulations suggest that biodegradation is an extremely complex and dynamic process with numerous interrelationships and influences existing between the entities of the landfill system. With further development, the model may be applied by landfill managers concerned with assessing landfill performance/impact over time and optimizing controllable parameters for biodegradation.

INVESTIGATION OF BIODEGRADATION PROCESSES IN SOLID WASTE LANDFILLS

I. Introduction

Historically, the landfilling of wastes has been viewed as a low-cost and limitless disposal option; as one landfill reaches its capacity, another one is built (Senior and others, 1990:93). Several factors have shifted the emphasis of landfill disposal away from this approach toward technological and management methods concerned with the long-term performance and capacity of landfills. The most influential factors include the increasing trend in the amount of solid waste generated over time, the decreasing number of existing landfills and difficulty in siting landfills, the environmental hazards associated with landfills, and the economic potential stemming from landfill operations. Because of the pressure these factors have exerted on solid waste management, both landfill operation and environmental impact have become significant issues facing both civilian and military communities.

Solid Waste Generation

According to a 1989 final report written by the Municipal Solid Waste Task Force from the Office of Solid Waste of the Environmental Protection Agency (EPA), the United States generates more solid waste per capita than any other nation and is projected to generate a total of approximately 190 million tons of municipal solid waste (MSW)

annually by the year 2000 (EPA, 1989:1-6). As of 1992, roughly 70% of the waste (150 million tons) was disposed in landfills (Ham and others, 1992:1486). In 1994, an updated EPA solid waste document reported 207 million tons of MSW generated in 1993 and estimated 218 million tons would be produced annually by the year 2000 (EPA, 1994:3-4). Of the 207 million tons produced, the EPA states that 129 million tons or 62% were landfilled in 1993 (EPA, 1994:4). A yet-to-be published 1995 EPA report with the most current EPA solid waste estimates states that 209 million tons was produced in 1994 with 127 million tons or 61% landfilled (EPA, 1995:5-6). Even with 30% of the waste diverted through recycling and composting, the EPA still predicts 118 to 122 million tons will be landfilled annually by the year 2000 (EPA, 1994:4; EPA, 1995:9-11).

The generation of MSW is clearly increasing over time and, even though the tonnage disposed in landfills has recently been decreasing, the EPA emphasizes landfilling will remain the *predominant* MSW management method in the future with landfill tonnage increasing to 132 million tons by 2010. (EPA 1995:5,11) It must also be noted that the decreasing landfill tonnage numbers estimated by the EPA assume certain percentages of waste diverted or recycled, and these percentages may or may not remain valid in the future (EPA, 1994:4; EPA, 1995:4). Ultimately, even if effective waste management through source reduction and recycling can reduce the amount of waste which eventually ends up in a landfill, there remains a significant portion of wastes still requiring landfill disposal. Until environmentally preferable, economically viable alternatives to landfill disposal are developed, landfilling wastes will remain the primary and most popular means of waste disposal (Ham and others, 1992:1486).

Landfill Assessment

Federal and state regulations and public resistance to landfill siting have been largely responsible for the decline in the number of both existing and planned landfills. Regulations were enacted to address the potential environmental hazards associated with landfills. The federal regulations address issues ranging from location restrictions and operating criteria to groundwater monitoring and postclosure care. States implement these regulations, and several states enforce even stricter regulations on landfill operations. Unable to comply with the stipulations of the Resource Conservation and Recovery Act (RCRA), Subtitle D, and the EPA Regulations on Criteria for Classification of Solid Waste Disposal Facilities and Practices (40 CFR 258) many landfills were forced to close causing a decline of 62% in the number of operating landfills from 7575 landfills in 1988 as estimated by General Accounting Office to 2893 in 1995 as estimated by the National Solid Waste Management Association (Blakely and Repa, 1996:171-172).

As public environmental awareness has grown over the years, so has the difficulty in landfill siting. The public is better informed today on the potential hazards associated with landfill operations. Public concerns center on the environmental and health impacts of a landfill, but may also include the odor and noise associated with a landfill, property values, equity issues arising from landfill siting, etc. (EPA, 1989:1-6). Public resistance culminates with the "Not In My Backyard" (NIMBY) syndrome and results in fewer places available to site landfills (EPA, 1989:1-6).

Environmental Hazards

A solid waste landfill can be characterized as a biochemical reactor wherein the waste materials degrade, producing landfill gas and altering the amount and composition of liquids (leachate) present in the landfill. The leachate produced by landfill biodegradation may contain contaminants such as heavy metals and trace organics or pathogens with the potential for human health risks (Tchobanoglous and others, 1993:428-429). If leachate is not properly managed or a landfill's lining system does not maintain its integrity, the leachate may eventually reach the water table possibly contaminating the groundwater. As of 1986, almost 50% of the operating landfills were within 1.6 km of a drinking water well. Most of these landfills were constructed without a landfill liner or leachate collection system (Barlaz and Palmisano, 1996:19). Such potential for contamination is an obvious concern for regulators and the public alike.

The major environmental problems arising from landfill gas include odors, explosions and fires, and groundwater acidification (Senior and others, 1990:93-94; Nyns and Gendebien, 1993:254). Landfill gases (primarily methane and carbon dioxide) are acknowledged greenhouse gases, potential contributors to the controversial global warming problem (Boeckx and Van Cleemput, 1996:189; Chynoweth, 1996:9-12; Masters, 1991:421-422).

Economic Benefits

Although a landfill gas such as methane can have potentially hazardous environmental and health effects, it can also generate economic benefits through energy recovery. The methane gas produced by landfill degradation can be captured and utilized

for energy purposes. Table 1 illustrates one of several depictions of the practical energy potential of methane gas generated by landfill biodegradation (Note that although the European Community (EC) produces more solid waste than the United States, the EC has less potential landfill gas because several countries of the EC landfill less than 67% of their waste as compared to 80% for the U.S.).

Table 1. Practical Yearly Potential of Landfill Gas from Domestic Solid Waste

			Annual Energy Potential	
Region	**Solid Waste (10^6 tons/yr)**	**Potential Landfill Gas (m^3/year)**	**Oil Equivalent (10^3 tons/yr)**	**TJoules (10^3/yr)**
United Kingdom	28	2520	1189	49.8
United States	165	13.2×10^3	6227	261
European Community	183.3	12.5×10^3	5896	247

Nyns and Gendebien, 1993:257

It has been estimated that 1% of the total United States energy needs could be met by the utilization of landfill gas (Senior and others, 1990:94). Unfortunately, the heterogeneity of landfill degradation has prevented the exploitation of landfill gas on a widespread basis. Energy recovery projects are abandoned due to the unpredictability of both the onset and subsequent future yields of methane production (Barlaz and others, 1989:1088; Barlaz and others, 1992:257). Only the largest landfills, with the ability to extract enough landfill gas to offset the gas generation fluctuations, can turn the recovery of landfill gas into an economically viable energy project.

Approaches to Assessing Landfill Performance and Environmental Impact

The performance of a landfill may be viewed from two different perspectives: as a cell or containment vessel, for which performance is measured in terms of its ability to isolate its contents from the environment, or as a biochemical reactor which concentrates on processes occurring within the landfill itself (See Figure 1.).

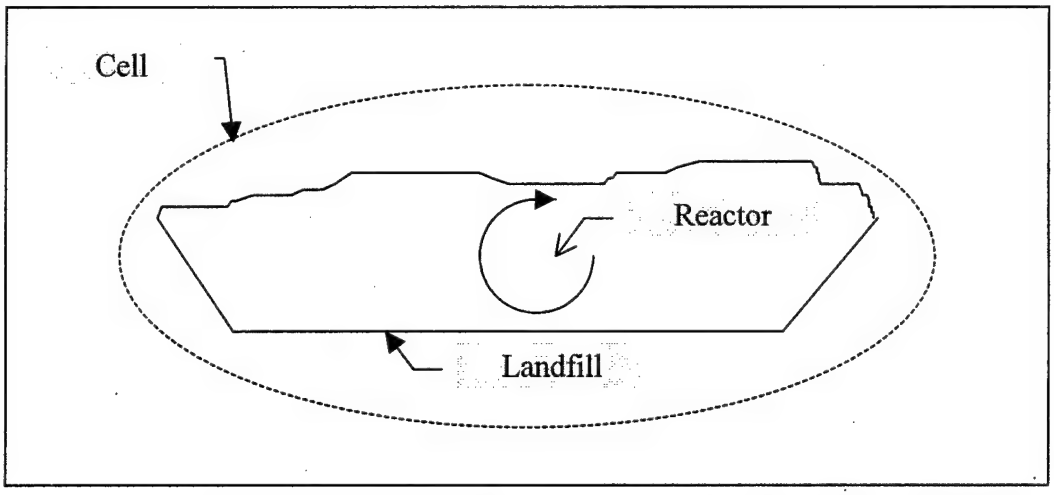


Figure 1. The Cell and Reactor Aspects of a Landfill

In conjunction with the cell and reactor perspectives, two different philosophies have emerged in constructing and managing landfills. Mandated by regulations aimed at minimizing their environmental impact, landfills have become tighter hydrogeologic structures providing greater waste isolation from moisture influx and transport (Bogner, 1992:104). Through the use of liners, compacted covers, and leachate collection, such structures remain "dry tombs" precluding the rapid biodegradation of waste contained within the landfill. The goal of this "dry-tomb landfill" philosophy is to maintain landfill

integrity in hopes of preventing or minimizing the production and/or escape of landfill gas and leachate. Accordingly, the approach concentrates on identifying and managing factors affecting the landfill as a containment vessel or cell. While this philosophy may lower landfill gas generation and leachate rates, it also has several disadvantages to include increasing the time required to completely degrade the waste, extending the duration of gas and leachate generation, and allowing gas and leachate generation times to exceed containment and treatment equipment service life.

Currently, there are several different models available to replicate the performance of landfills from a cell perspective based on various external parameters responsible for landfill failure such as water infiltration, cell design, site proximity to wells or aquifers, and contaminant transport mechanisms. The list of models includes deterministic water balance models which predict leachate leakage through soil liners and covers, relative risk methodologies which use structured value systems to rank landfill sites according to the environmental hazards they pose, and stochastic simulation models which attempt to identify and quantify the magnitude and probability of occurrence of every contaminant release mechanism (Nixon and Murphy, 1995:2-8). An empirical model of landfill containment performance was also recently developed (Nixon, 1995). These models address the interaction of a landfill with its environment but not the *internal* longevity/capacity/energy production issues of landfill operation.

In contrast to the "dry tomb" approach, the "wet-cell" philosophy seeks to treat landfills as biodigestors designed to enhance microbial degradation processes (Wall and Zeiss, 1995:214). The goal is not landfill integrity but to ensure the conditions conducive

to faster biodegradation are present and maximized; thus, the "wet-cell" approach concentrates on processes within the landfill responsible for biodegradation of waste. Enhanced biodegradation reduces the stabilization time of landfills while reducing the amount of time liners must remain intact to prevent leachate and gas leakage thereby minimizing landfill environmental impacts (Wall and Zeiss, 1995:214). Accelerating biodegradation rates can also significantly increase the capacity of a landfill by amplifying the initial settlement of waste (Wall and Zeiss, 1995:222). Improved biodegradation can also generate the volumes of methane necessary to make energy recovery a viable economic project for the landfill (Bogner, 1990:330; Senior and others, 1990:93-94). Additionally, if degraded landfill material were to be mined for use in improving soils or recovery of recyclable materials, decreasing the cycle time between waste emplacement and material recovery could be achieved through accelerated degradation (Murphy and others, 1995:485).

To comprehensively assess landfill performance as a reactor, the microbiological, chemical, and physical processes responsible for the degradation of waste should be fully understood. However, the most significant process controlling decomposition is microbiological degradation (Murphy and Brennan, 1992:2). Understanding the causes and interactions behind the complex degradation processes and what variables are important (and when) for the process behavior could allow for the identification and manipulation of alternative actions which could control or enhance the process. The biological processes of a landfill could be managed to optimize long term efficiency of a

landfill and exploit the benefits associated with accelerated decomposition while minimizing environmental impacts, if the process behavior is understood.

Problem Statement/Thesis Purpose

To summarize, the United States faces increasing amounts of solid waste with fewer landfills to accept it. Landfill managers face greater demands on landfill capacity while trying to meet stricter regulations intended to minimize landfill environmental impacts. In optimizing the balance between the longevity/capacity of a landfill, the potential for environmental hazards, and the possible economic benefits of landfill operations, the "wet-cell" philosophy is gaining momentum as a viable alternative to the conventional "dry-tomb" approach for solid waste management. The key to managing the landfill effectively from the "wet-cell" viewpoint is first understanding the dynamic biodegradation processes associated with landfill operation, both in space and time.

The purpose of this thesis is to determine and explore the fundamental processes within the landfill biochemical reactor responsible for the degradation of municipal solid waste. Such an effort could serve as the foundation for models, which eventually would be utilized in future applications of landfill management concerned with assessing landfill performance/impact over time and optimizing controllable parameters for biodegradation. The ability to model landfill performance over time and determine optimal parameter values would allow landfill managers to effectively assess and manage their particular sites. Modeling landfill performance over time could also facilitate the determination of when a particular landfill will fail given the amount of time its containment system will last and the length of time required to degrade the remaining waste in the landfill. Other

examples of landfill management applications include the prediction of methane production and optimization of methane producing conditions (Barlaz and others, 1987:27). Conversely, the minimization of methane production at sites without effective gas collection systems might be better achieved through enhancement of the aerobic-stage degradation processes and conditions.

Scope/Limitations

Either leachate or landfill gas can be used in assessing landfill performance, but landfill gas constituent concentration and flux provide a more predictable metric commensurate with the dynamic behavior of the landfill biodegradation process. Thus, only landfill gas will be utilized as a metric of biodegradation in the thesis. Most importantly, the thesis will be limited to the factors essential to the degradation process based on the biochemical reactor aspect of a landfill. Although factors exterior to the landfill vessel may affect the parameters crucial to degradation such as moisture, boundaries have been established regarding the detail and scope of the model to stay focused on the mechanisms responsible for the overall biodegradation process itself due to the complexity of including external factors such as freeze/thaw cycles and climatic conditions.

II. Literature Review

General Progression of Biodegradation

In order to realistically model the fundamental processes of biodegradation associated with landfill disposal, it is necessary to first understand the general progression of the decomposition process. Although the fundamental processes of biodegradation have been aggressively studied by countless authors, it remains an extremely complicated subject. The heterogeneity of landfill conditions and bacterial species, as well as the complexity of microbial interactions associated with decomposition, result in explanations of the overall biodegradation process being limited to general descriptions in literature. The process is usually broken down into various phases which illustrate the time and event order for biodegradation with four, five or six phase sequences represented by the generation of landfill gases (Murphy and Brennan, 1992:2). Most process descriptions propose either a four or five-phase sequential approach.

The four-phase approach divides the biodegradation process into the following general phases: aerobic degradation, anaerobic acid, accelerated methane, and decelerated methane (Barlaz and others, 1989:1089-1090; Barlaz and Palmisano, 1996:37-45). The five-phase approach differs slightly by splitting the anaerobic acid phase into two different phases, transition and acid. The following general phases form the basis for the five-phase description: initial adjustment (I), transition (II), acid (III), methane fermentation (IV), and maturation (V) (Tchobanoglous and others, 1993:384-

387; Reinhart and Townsend, 1998:16-17). Figure 2 illustrates the landfill gas production for the four phases for a laboratory-scale experiment.

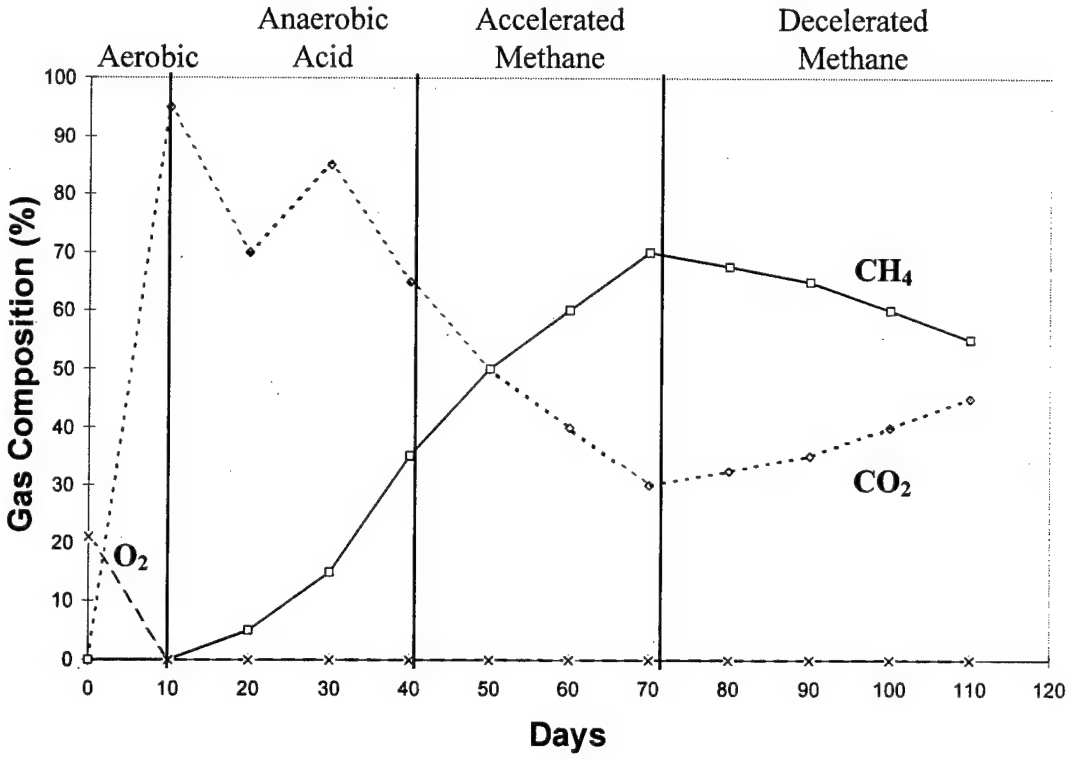


Figure 2. Four Phases of Decomposition and Landfill Gas Production (after Barlaz and others, 1989:1089; Barlaz and Palmisano, 1996:40)

Figure 3 depicts a theoretical illustration of landfill gas generation for five phases.

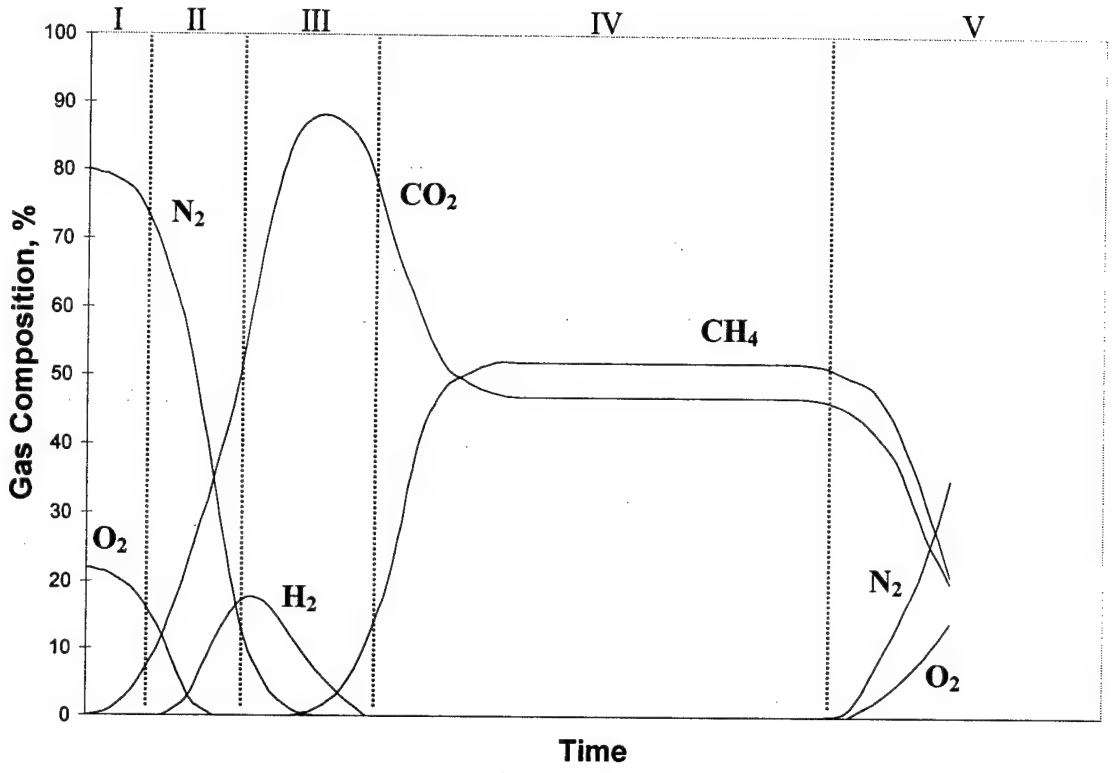


Figure 3. Theoretical Five Generalized Phases of Decomposition and Landfill Gas Production (after Tchobanoglous and others,1993:385)

Regardless of which approach is viewed as more appropriate, each of the sequences has three common phases: aerobic degradation; anaerobic decomposition that facilitates carbon dioxide and organic acid generation; and methanogenesis, which converts the products of anaerobic decomposition to methane and carbon dioxide (Murphy and Brennan, 1992:2). Table 2 summarizes the general phenomena associated with the degradation process as depicted by the phases of landfill gas generation (Barlaz and others, 1989:1089-1090; Tchobanoglous and others, 1993:384-.387; McBean and others, 1995:72-73).

Table 2. Summary of Landfill Gas Generation Phases

Four-Phase Approach	Five-Phase Approach	Phase Description
Aerobic	Initial Adjustment	Beginning of decomposition under aerobic conditions; O_2 depleted; CO_2 produced; normally lasts only a few days
---	Transition	O_2 completely depleted; anaerobic decomposition begins
Anaerobic Acid	Acid	Anaerobic decomposition; organic acids accumulate; CO_2 principal gas generated; H_2 also produced; pH decreases
Accelerated Methane	Methane Fermentation	Rapid accumulation of methane; CO_2 also produced; organic acids consumed; pH increases; duration can vary from 3 months to years
Decelerated Methane	Maturation	Production of methane remains steady until organic matter is depleted

Aerobic Degradation. The general aerobic transformation of organic waste is depicted with the following equation (Tchobanoglous and others, 1993:677).

$$\text{Organic Matter} + O_2 + \text{nutrients} \xrightarrow{\text{Bacteria}} \text{new cells} + \text{resistant organic matter} + CO_2 + H_2O + NH_3 + SO_4^{2-} + \ldots + \text{heat}$$

During aerobic degradation the oxygen present during burial of refuse is consumed with the available organic waste serving as the source of aerobic microbial activity. Oxygen serves two different functions during degradation: a terminal electron acceptor of

electrons released during oxidation of organic carbon and a reactant in the attack on substrate molecules (Schink, 1988: 775).

Although aerobes initiate the overall degradation process, they play a minor role in refuse decomposition and landfill gas production as a whole. (Barlaz and Palmisano, 1996:9). The aerobic or initial adjustment phase normally lasts only a few days, depending on other refuse conditions such as moisture content (McBean and others, 1995:72). After oxygen depletion, roughly 98% of the soluble sugars remain (Barlaz and others, 1989:1099). Landfill gas composition during this phase is nearly 100% carbon dioxide (Barlaz and Palmisano, 1996:42).

Two important factors of the landfill ecosystem are generated during this phase: heat and moisture. Aerobic decomposition generates heat with a possible temperature rise of 10 to 20 deg C above ambient temperature (McBean and others, 1995:72). Such heat generation is important in providing the temperature range to maintain anaerobic digestion (Archer and Robertson, 1986:118). The addition of moisture is also crucial in providing the proper environmental conditions for the anaerobic bacteria to carry out further degradation of organic material.

Compared to anaerobic bacteria, aerobes are more efficient in utilizing organic material for energy. Oxygen-based microbial metabolism is more efficient than fermentation with high energy availability following the introduction of waste (Barlaz and Palmisano, 1996:133; McCarty, 1972: 102). During the anaerobic process, very little of the substrate energy is utilized for cell use with most of the energy remaining bound up in the products of each anaerobic degradative step (Mah, 1982:152). As a result of this

efficiency, aerobic degradation provides greatly enhanced decomposition as compared to anaerobic degradation (Murphy and Stessel, 1992:499).

Although several groups of bacteria are strictly anaerobic in nature (unable to survive in a strictly aerobic environment), all of the trophic groups of bacteria required for methanogenesis are present in fresh refuse; however, during this phase, their populations change very little (Barlaz and others, 1989:1089). Once the oxygen is depleted, the anaerobic bacteria can thrive, and subsequently, the anaerobic decomposition process can begin.

Anaerobic degradation. Anaerobic degradation incorporates the anaerobic acid or transition phase through decelerated methane or maturation stages. The general anaerobic transformation of organic waste is described with the following equation (Tchobanoglous and others, 1993:681).

$$\text{Organic matter} + H_2O + \text{nutrients} \xrightarrow{\text{Bacteria}} \text{new cells} + \text{resistant organic matter} + CO_2 + CH_4 + NH_3 + H_2S + \text{heat}$$

Although not depicted with this general equation, much like aerobic degradation, some portions of anaerobic decomposition such as methanogenesis generate moisture as well as heat. However, little heat is released during anaerobic metabolism (Archer and Robertson, 1986:120), and certain reactions in the anaerobic process such as hydrolysis consume moisture. Again, the importance of these factors in allowing the decomposition

process to continue stems from providing the necessary environment for the microbes to flourish.

An alternative representation of the entire anaerobic decomposition process can be summarized with the degradative steps which drive each phase of anaerobic decomposition. The relationship between the various anaerobic organisms responsible for each step reflect the interaction between each group of organisms. The products of one group of organisms serve as the substrate for another group. The different types of microbes are lined up with their catabolic activities to form an anaerobic food chain (Gottschalk, 1986:265). The nature of the end products depends on the microbial species involved and the environmental conditions present (Sawyer and others, 1994:298). Figure 4 lists each step and the products they produce.

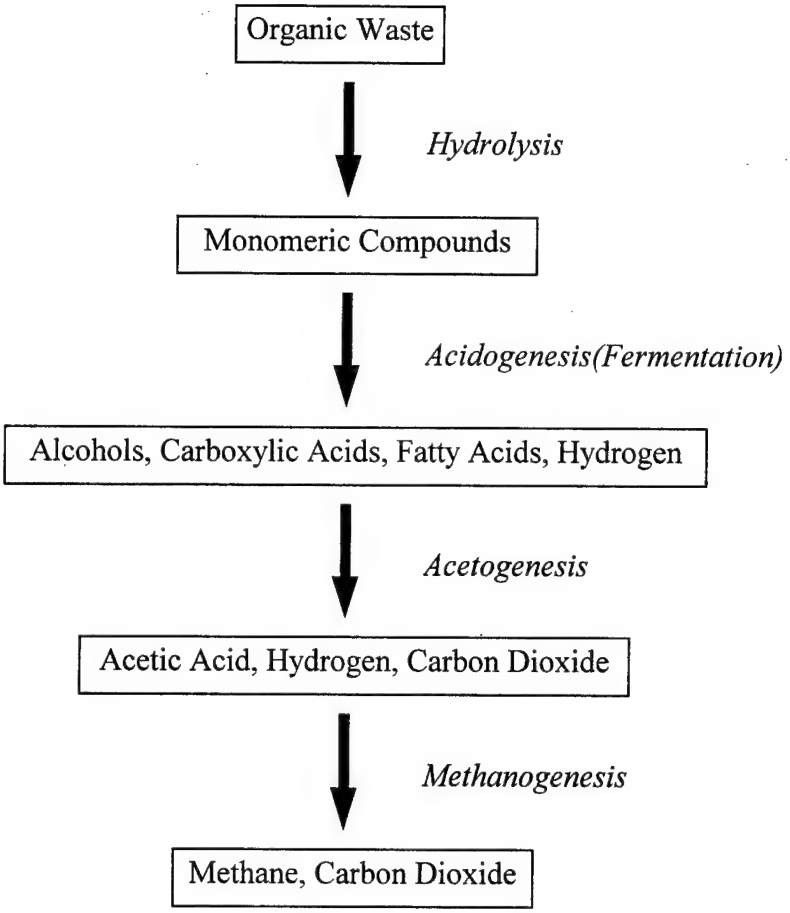


Figure 4. Major Degradative Steps of Anaerobic Degradation (after El-Fadel and others, 1996:310)

Barlaz ties the degradative steps and type bacteria responsible for each step in his summation of the anaerobic process in Figure 5.

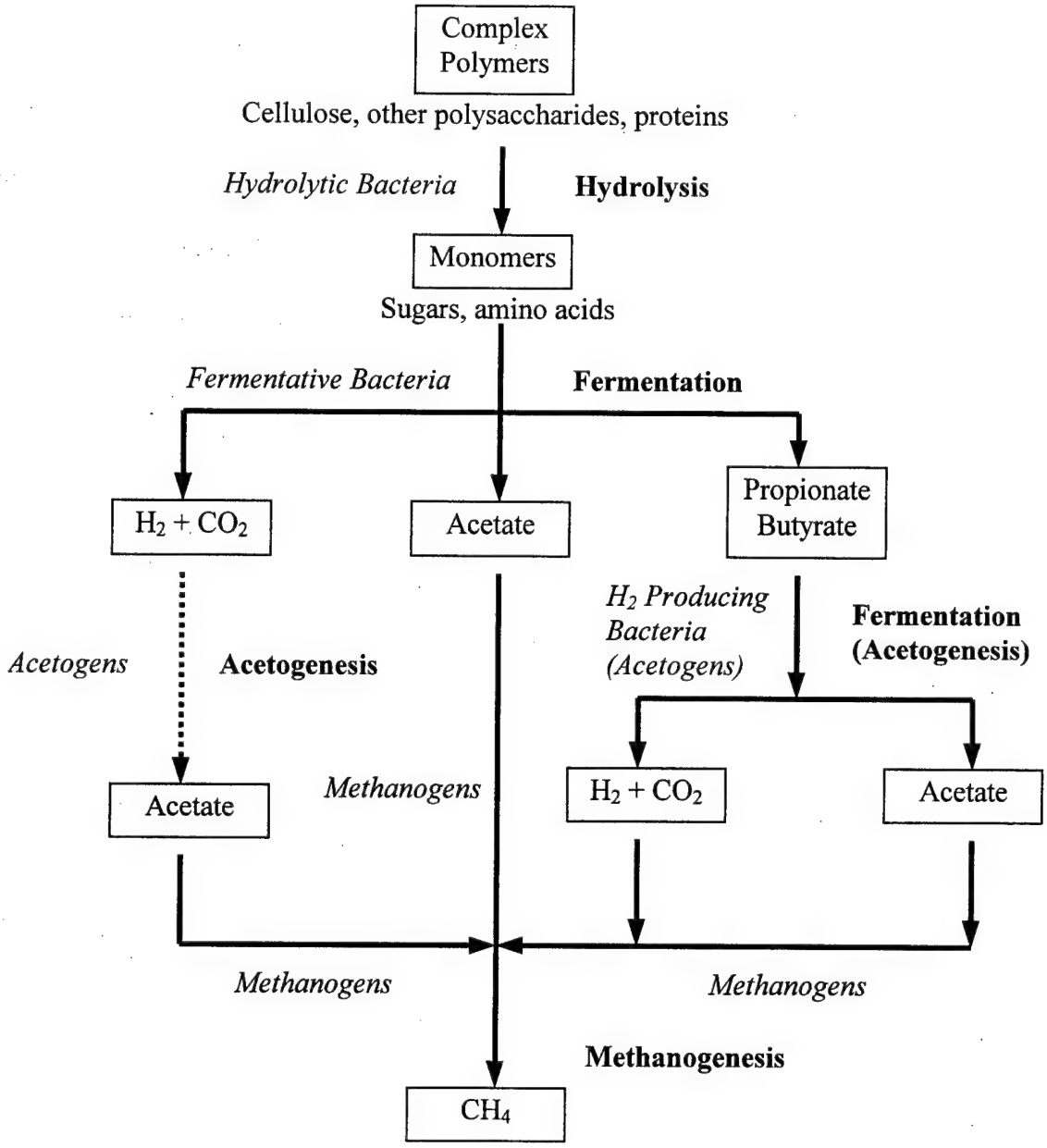


Figure 5. Anaerobic Decomposition by Consortia of Anaerobic Bacteria (after Barlaz and Palmisano, 1996:38)

Acetogenesis of hydrogen and carbon dioxide into acetate (as denoted by the dotted line in Figure 5) has not been established in the MSW landfill ecosystem (Barlaz

and Palmisano, 1996:39). Note that the authors differ in their interpretation of the conversion of acids to hydrogen, carbon dioxide, and acetate. Yet, different kinds of fermentations are identified by the major end products formed, so acetate-forming microorganisms have been generally identified as acetogens but there are types which also produce hydrogen and carbon dioxide (Gottschalk, 1986: 210; Dolfing, 1988:418). Acetogenesis can be considered a type or stage of fermentation (Bryant, 1979:194). Thus, neither author is inaccurate in assessing the overall anaerobic process. Table 3 depicts the phases and how they correspond to the degradative steps.

Table 3. Relationship of Landfill Gas Phases to Degradative Steps

Four Phases	**Five Phases**	**Degradative Step**
Aerobic	Initial Adjustment	Aerobic Degradation
---	Transition	Begin Hydrolysis, Begin Fermentation
Anaerobic Acid	Acid	Hydrolysis, Fermentation, Begin Acetogenesis and Methanogenesis
Accelerated Methane	Methane Fermentation	Hydrolysis, Fermentation, Acetogenesis, Methanogenesis
Decelerated Methane	Maturation	Reduced Hydrolysis, Fermentation, Acetogenesis, and Methanogenesis

It cannot be understated that the anaerobic portion of decomposition consists of numerous complex interactions and sequential events between numerous possible groups of anaerobic bacteria. For every stage of decomposition such as hydrolysis, each of the

separate reactions involved in completing the particular degradative step are complex processes which involve many different kinds of anaerobic microorganisms whose presence varies depending on the particular ecosystem and its conditions (McInerney, 1988:402). Such complexity is evident in the fact that although the major components of gaseous product being generated by anaerobic processes are carbon dioxide and methane (and hydrogen to a lesser degree), the actual gaseous product of anaerobic degradation can consist of 80 components depending on the refuse and landfill conditions (Senior and others, 1990:94).

Hydrolysis. The initial step of the anaerobic process is hydrolysis or the breakdown of complex substances into simpler substances which are suitable for use by the microorganisms. It is a substitution reaction where water acts as a nucleophile and is the most common substitution reaction catalyzed by microorganisms (Sawyer and others, 1994:272,310). During decomposition, hydrolysis occurs in more than a single reaction; complex substances are first hydrolyzed to simpler polymers such as carbohydrates and proteins which are further hydrolyzed to substances such as amino acids, simple sugars, and fatty acids (Bryers, 1985:638). The species of anaerobic bacteria which receive energy from growth by hydrolyzing complex polymers are collectively referred to as hydrolytic bacteria. Being the first step of the acid phase of the anaerobic process, it has been hypothesized that hydrolysis of complex organic materials to soluble substrates can be the rate limiting step in the acid phase of anaerobic digestion (Eastman and Ferguson, 1981:360).

Fermentation. The products of hydrolysis are converted directly to acetic acid or into lower molecular mass intermediate by-products such as carboxylic acids, acetic acid, other organic acids, and alcohols. The production of organic acids during this step affects the pH of the system, often lowering the pH of the waste if the buffering capacity of the waste is exceeded or the activity of the fermentative organisms exceeds the consumption activity of the acetogens and methanogens (Sawyer and others, 1994:298; Barlaz and Palmisano, 1996:43-44). Such a lowering of the pH may be detrimental to methanogens (Senior and others, 1990:101). In fermentation, biological processes occur without the involvement of oxygen or nitrate as the electron acceptor, instead the organic material being converted serves as the terminal electron acceptor (Gottschalk, 1986:208-210). There are numerous fermentation pathways along with the corresponding types of bacteria with the type of fermentation determined by its end-product. Carbon dioxide is the principal gas generated during this phase, with smaller amounts of hydrogen produced as well (Tchobanoglous and others, 1993:386). Bacteria that obtain energy from the fermentation processes are collectively referred to as fermentative bacteria.

Acetogenesis. Acetogenesis, a type of fermentation process, transforms the products of fermentation into acetate, hydrogen, and carbon dioxide. Consequently, CO_2 and H_2 are the gases generated during acetogenesis. The organic products of the preceding fermentation reactions are utilized as the terminal electron acceptors for this degradative step. Acetogens, strict anaerobes, accomplish this transformation only if these products, particularly hydrogen, are removed by methanogens as they are formed;

the conversion is only thermodynamically favorable at low hydrogen concentrations (Barlaz, 1988:5). Acetogens and methanogens maintain a unique balancing act to create conditions favorable for either acetogenesis or methanogenesis which simultaneously allows both processes to function properly. This relationship is often syntrophic in nature, meaning both partners rely on each other to perform their metabolic activities.

Methanogenesis. Methanogenesis is the terminal step in the anaerobic food chain. The substrate spectrum for methanogens (collective name for all bacterial species which obtain energy through methanogenesis) is relatively small compared to other fermentative bacteria consisting only of $H_2 + CO_2$, formate, methanol, methylamines, and acetate (Gottschalk, 1986: 265; Oremland, 1988:651). From these substrates, two independent pathways are generally associated with methanogenesis: the reduction of CO_2 with electrons from the oxidation of H_2 or fermentation of acetate to methane and CO_2 (Ferry, 1993:305). Estimates ranging from 65% to 75% have been cited for the production of methane from acetate during the degradation of organic material (Bryant, 1979:195; Van Den Berg and others, 1976:1312; Allen and Zinder,1996:275). Clearly, methane gas is generated during methanogenesis; however, carbon dioxide is also produced from the acetate pathway while also being consumed as a substrate for the other methanogenesis pathway. As the acetogens and methanogens work to transform and consume the organic and acetic acids, the pH within the landfill will rise to more neutral values. Methanogens are obligate anaerobes and extremely sensitive to even low levels of oxygen (Gottschalk, 1986:252; Oremland, 1988:655).

Stoichiometric Relationships of Biodegradation

Each step in the degradation process, and subsequently each phase of landfill gas generation, has biochemical equations associated with it that depict the reactions responsible for substrate utilization in the step and the products each step generates. The following stoichiometric equation is an overall representation of biodegradation and generation of landfill gas (Tchobanoglous and others, 1993:388; Barlaz and others, 1989:1094).

$$C_aH_bO_cN_d + ((4a - b - 2c + 3d)/4)H_2O \xrightarrow{\text{Bacteria}} ((4a + b - 2c - 3d)/8)CH_4 + ((4a - b + 2c + 3d)/8)CO_2 + dNH_3$$

Although this general equation is often used to predict the methane potential of various types of wastes (Barlaz and others, 1989:1094), the equation only addresses the beginning and end of the degradation process.

With countless major and intermediate reactions possible in such a complex process as biodegradation, no comprehensive and exhaustive list of reactions exists, so the following stoichiometric equations represent equations aggregating the degradative steps from known documented biochemical equations. The compositions of the generic organic waste and other substrates chosen for the stoichiometry of the decomposition process were a result of balancing these aggregated equations accordingly.

Aerobic Degradation. During the aerobic phase of decomposition, two basic reactions occur: hydrolysis by aerobes, and aerobic degradation of simpler substances.

$$C_{16}H_{34}O_{13} + O_2 + 3H_2O \xrightarrow{\text{Aerobes}} 2C_8H_{18}O_7 + 4OH \qquad \text{Hydrolysis}$$

$$C_8H_{18}O_7 + 9O_2 \xrightarrow{\text{Aerobes}} 8CO_2 + 9H_2O \qquad \text{Aerobic Degradation}$$

The initial hydrolysis equation is based on both oxygen and water being available for aerobic hydrolysis to be completed. The aerobic degradation equation is predicated on the following basic stoichiometric equation describing aerobic growth on simple substances frequently cited in microbiological literature (Gottschalk, 1986:12; Sawyer and others, 1994:298; Archer and Robertson, 1986:120).

$$C_6H_{12}O_6 + 6O_2 \xrightarrow{\text{Aerobes}} 6CO_2 + 6H_2O \qquad \text{Aerobic Degradation}$$

In both aerobic reactions, the aerobes directly influence the rate at which the reaction occurs. As evident from the equations, CO_2 and moisture are the major end-products of the aerobic phase.

Anaerobic Degradation. Anaerobic degradation begins with hydrolysis but with no oxygen required for the reaction. The initial organic waste composition remains the same for hydrolysis.

$$C_{16}H_{34}O_{13} + H_2O \xrightarrow{\text{Hydrolytic Bacteria}} 2C_8H_{18}O_7 \qquad \text{Hydrolysis}$$

Much like aerobic hydrolysis, water is required for hydrolysis, regardless of the presence of oxygen. For this type of hydrolysis, the hydrolytic bacteria drive the reaction.

Once soluble organic materials become available to other microorganisms, fermentation of the simpler substances occurs with fermentative bacteria influencing the reaction. Knowing that fermentation produces certain end-products, the following stoichiometric equation was derived and balanced given the same simpler substance composition as seen in aerobic degradation.

$$C_8H_{18}O_7 \xrightarrow{\text{Fermentative Bacteria}} \left.\begin{array}{l} CH_3CH_2OH\text{(alcohol)} + CO_2 + H_2 + \\ H(CH_2)_2COOH\text{ (carboxylic acid)} + \\ CH_3COOH\text{ (acetate)} \end{array}\right\} \text{Fermentation}$$

(Gottschalk, 1986: 208-260)

With fermentation end-products now available, the acetogens can now drive various forms of acetogenesis. Note that acetogenesis can also form additional acids from alcohols present. The acids and alcohols are ultimately converted to acetate.

$$\left.\begin{array}{l} H(CH_2)_2COOH + 2H_2O \xrightarrow{\text{Acetogens}} 3CH_3COOH + 2H_2 \\ CH_3CH_2OH + H_2O \xrightarrow{\text{Acetogens}} CH_3COOH + 2H_2 \\ CH_3(CH_2)_2OH + H_2O \xrightarrow{\text{Acetogens}} H(CH_2)_2COOH + 2H_2 \end{array}\right\} \text{Acetogenesis}$$

(Young, 1995:71-72; Mah, 1982:606; Gottschalk, 1986: 208-260; Dolfing, 1988:426)

Finally, once the substrates required for methanogenesis are made available from previous degradative steps, the following reactions involving methanogens can occur:

$$CH_3COOH \xrightarrow{\text{Methanogens}} CH_4 + CO_2$$

$$CO_2 + H_2 \xrightarrow{\text{Methanogens}} CH_4 + 2H_2O$$

} Methanogenesis

(Muller and others, 1993:360-396; Ferry, 1993:309-310; Gottschalk,1986:252-260; Oremland, 1988:651; Vogels and others, 1988:709; Chynoweth, 1996:7; Barlaz and Palmisano, 1996:81)

It must be emphasized that these stoichiometric equations are *not* comprehensive in nature. Certainly, there are numerous intermediate reactions not represented by these equations and some reactions presently undiscovered. These equations are employed for this thesis based on the literature available, frequency of use in literature, literature study of the degradative steps themselves and their reactants and products, and the knowledge that these particular equations appear to capture the majority of the primary reactions involved in the decomposition process.

Bacterial Growth

Clearly biodegradation relies on microorganisms to carry out the process, so it is advantageous to understand the basic principles of bacterial growth. Bacterial growth

based on mass of microorganisms can be summarized with the following four phases (Metcalf and Eddy, 1991:367-368; Reynolds, 1982:260-263):

1. The lag phase ---	Bacteria require time to adjust to their environment. The lag phase duration will depend on the initial conditions of the environment. The lag and log-growth phases are often combined when dealing with mass based growth.
2. The log-growth phase ---	Conditions are extremely favorable for the bacteria with plenty of substrate available. The rate of growth is only limited by the bacteria's ability to process substrate.
3. Declining growth phase ---	Towards the end of the log-growth phase, growth becomes limited due to the depletion of substrate or essential nutrient, or the accumulation of an inhibitory substance. When the mass of bacteria being produced equals the decrease in mass, the curve peaks.
4. Endogenous phase ---	In this phase, the microbes are forced to metabolize their own food stores or protoplasm due to the shortage of substrate.

Figure 6 is a graphical representation of the phases of bacterial growth based on the mass of cells.

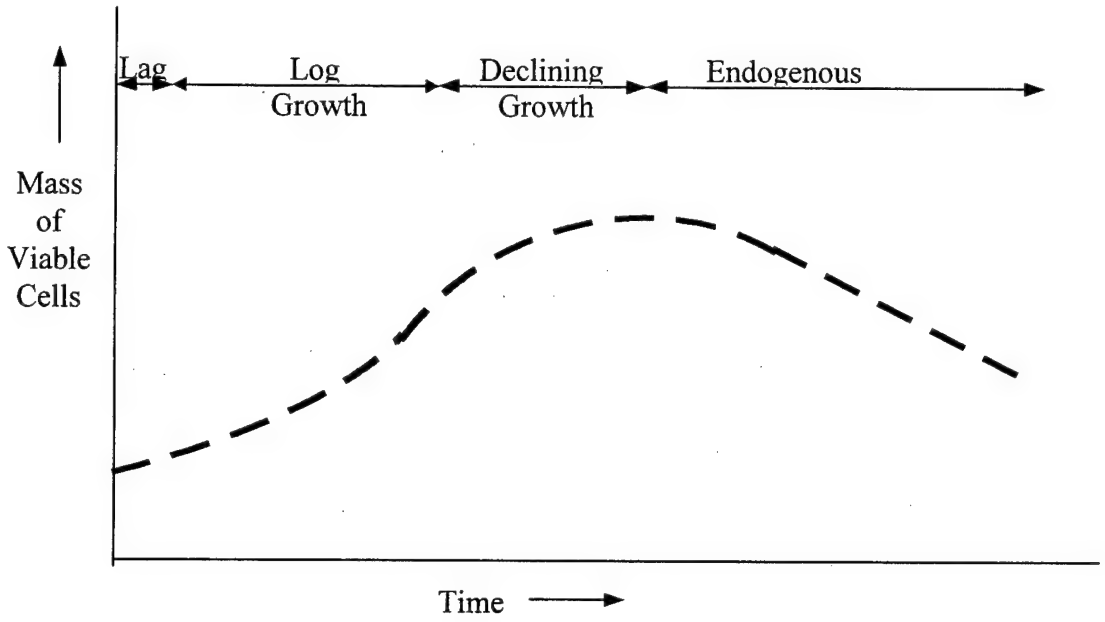


Figure 6. Microbial Growth Phases Based on Bacterial Mass (after Metcalf and Eddy, 1991:367-368; Reynolds, 1982:260-263)

Kinetics of Microbial Growth. The rate of growth of bacteria can be defined with the following relationship in which the rate of increase of the concentration of microorganism is proportional to the microorganism concentration (Metcalf and Eddy, 1991:370; Gaudy and Gaudy, 1980:232).

r_g or $dX/dt = uX$ where r_g or dX/dt = rate of bacterial growth (mass/unit vol x time)

u = specific growth rate ($time^{-1}$)

X = concentration of microorganism (mass/unit vol)

Substrate limited growth can be adequately described using the following equation first derived by Jacques Monod (Metcalf and Eddy, 1991:370; Monod, 1949:383-384).

$u = u_m(S/(K_S + S))$ where u = specific growth rate ($time^{-1}$)

u_m = maximum specific growth rate ($time^{-1}$)

S = concentration of substrate (mass/unit vol)

K_S = half-saturation constant, substrate concentration at one-half the maximum growth rate (mass/unit vol)

Thus, r_g or dX/dt becomes

r_g or $dX/dt = u_m X(S/(K_S + S))$

Figure 7 illustrates the effect of a limiting substrate on the specific growth rate of bacteria (Metcalf and Eddy, 1991:371).

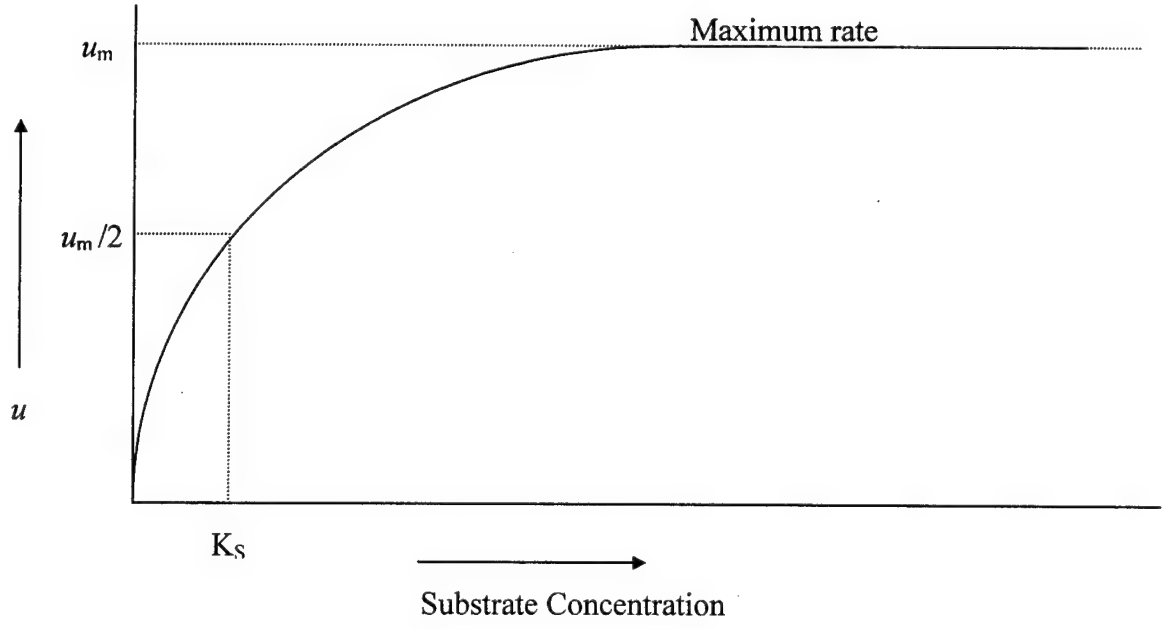


Figure 7. Plot of Specific Growth Rate vs. Substrate Concentration

For microbial populations which have two substrates able to limit growth, the following expression was derived (Bader, 1982:11).

$$r_g \text{ or } dX/dt = \frac{u_m X S_1 S_2}{(K_1 + S_1)(K_2 + S_2)}$$

To describe the "death" of microbial mass, the decrease in mass is considered proportional to the concentration of organisms present (Metcalf and Eddy, 1991:372).

r_d (endogenous decay) $= -k_d X$ where k_d = decay coefficient (time^{-1})

X = concentration of cells (mass/unit vol)

Bacterial growth will be influenced by various conditions of the microorganism's environment. These conditions will often determine whether the bacteria have the proper conditions for growth. As these factors influence the microbial populations responsible for degradation and landfill gas generation, the entire decomposition process is affected.

Environmental Factors Influencing Biodegradation

Biodegradation and, subsequently landfill gas generation, are influenced by numerous environmental factors to include moisture content, pH, waste temperature, waste type, refuse density, site operational factors, and nutrients (Pacey, 1986:51). Most of these factors prove influential because of their impact on the microorganisms driving the degradation process itself. Figure 8 illustrates the parameters affecting methane

generation, although most of these parameters will affect other degradative steps and gas generation.

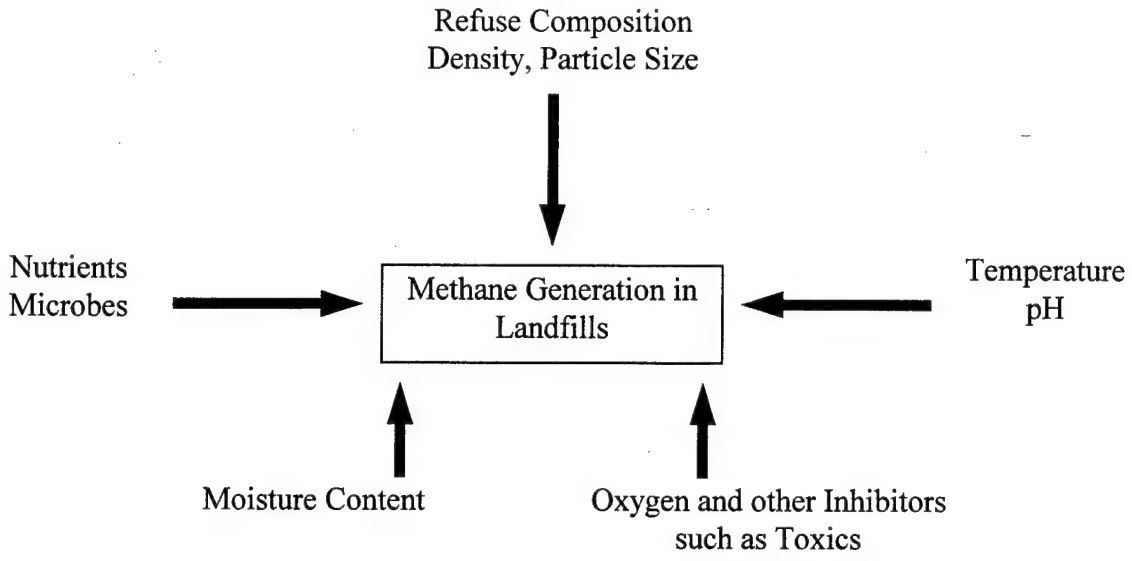


Figure 8. Factors Influencing Methane Generation in MSW Landfills (after (El-Fadel and others, 1996:313)

Although there are even more factors which could be listed, the most influential factors in degradation according to available literature appear to be moisture content, pH, temperature, nutrients, and the presence of oxygen (for the anaerobic stages). Several authors note the strongest influences and correlation between gas generation and these parameters when researching the effects of various parameters on degradation (Barlaz and others, 1990:569-575; Barlaz and Palmisano, 1996:93-100; Pacey, 1986:51-54; El-Fadel and others, 1996:314; Van Den Berg and others, 1976:1315; Young, 1995:73-81).

Moisture Content. Moisture content of refuse is derived from three different sources: initial moisture content of the waste, moisture infiltration from outside the

landfill, and moisture generated by microbial catabolic activity (Senior and others, 1990:96). Moisture content is considered the most important parameter affecting decomposition and subsequent landfill gas generation (McBean and others, 1995:73). Degradative bacteria require moisture to survive. Moisture provides the aqueous environment essential for microbial digestion while facilitating the distribution of bacteria and nutrients within the landfill. Consequently, bacteria thrive as moisture content increases. A moisture content of at least 50% is considered desirable for methanogenesis to occur (Gurijala and Suflita, 1993:1178). The range of the moisture content of refuse received at landfills typically varies from 15 to 40 percent on a wet weight basis (McBean and others, 1995: 75).

pH. Anaerobic degradation is characterized by changes in pH as a result of fermentation, acetogenesis, and methanogenesis. As fermentation occurs, the pH decreases until the acidic fermentation products are utilized by the acetogens and methanogens causing an increase in landfill pH. Low pH values resulting from the accumulation of organic acids can inhibit methanogenesis.

The ideal pH range for methanogenesis ranges anywhere from 6.4, 6.7, or 6.8 to 7.2 or 7.4 depending on the author cited and whether the information was derived from laboratory or field experimentation (Gurijala and Suflita, 1993:1180; Bryant, 1979:199; Barlaz and others, 1990:575). Figure 9 illustrates a normalized curve of the optimal pH range for methanogenesis.

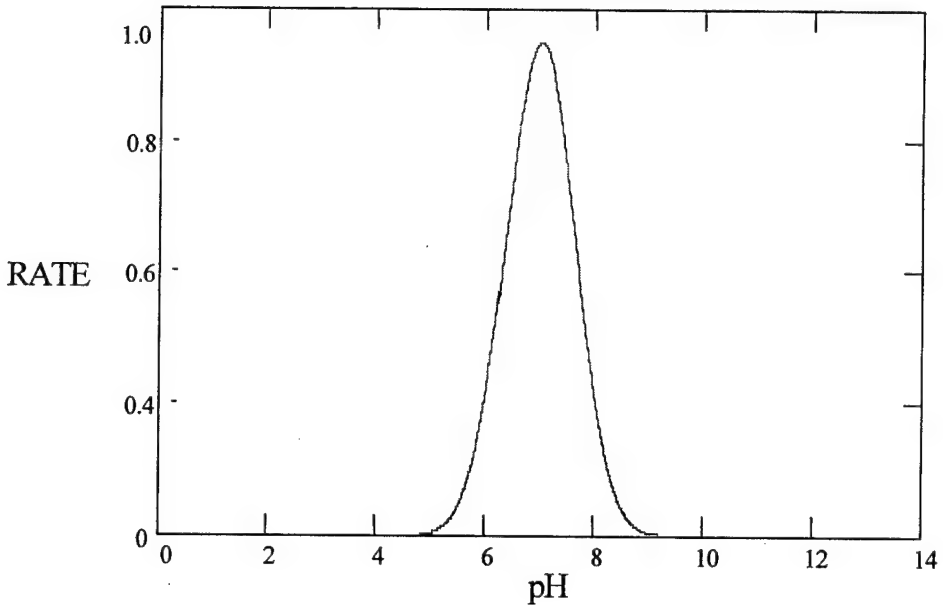


Figure 9. Normalized Curve of Methanogenesis vs. pH (afterYoung, 1995:78).

Outside these ranges (roughly below 6 or above 8), methanogenesis can be severely limited (McBean and others, 76; Bryant, 1979:199). Nonetheless, some studies indicate that methanogens can survive and function in rather acidic conditions or conditions above a pH of 8 (Kasali and others, 1988:231; Grahame and Stadtman, 1993:348-350). Initial pH values for actual landfill samples indicate values above neutral; however, these values can fluctuate tremendously depending on waste composition and landfill conditions (Jones and others, 1983:243).

Temperature. According to the temperature range in which they thrive, bacteria can be classified into the following categories in terms of temperature as seen in Table 4 (Tchobanoglous and others, 1993:676).

Table 4. Typical Temperature Ranges for Bacteria

Type	Temperature, deg C	
	Range	Optimum
Psychrophilic	-10 to 30	15
Mesophilic	20 to 50	35
Thermophilic	45 to 75	55

Other authors quote slightly different optimum temperatures for the bacteria: 30 to 35, 20 to 45, or 25 to 40 deg C for mesophilic and 45, 45 or above, and 55 to 65 deg C for thermophilic (McBean and others, 1995:63; Gaudy and Gaudy, 1980:177-178; Metcalf and Eddy, 1991:366).

According to laboratory studies of decomposition, temperature appears to be a major factor in controlling gas generation in landfills (Hartz and others, 1982:635). In general, microbial metabolic activity and landfill gas generation increase with increasing temperature (Atlas and Bartha, 1993:219; El-Fadel and others, 1996:314). As microbial activity increases, the heat given off by microbial degradation reactions raises the temperature. The rise in temperature causes increased microbial activity. Bacterial growth rates or enzyme activity can double with approximately every 10 deg C increase in temperature until the optimum temperature is reached (Tchobanoglous and others, 1993:676; Metcalf and Eddy, 1991:365; Atlas and Bartha, 1993:219). However, temperatures below the optimum usually impact growth rates greater than temperature increases above the optimum (Metcalf and Eddy, 1991:365).

Low temperatures can affect degradation by slowing down microbial activity. High temperatures can eventually exceed bacterial tolerance for temperature leading to the cessation of microbial activity and gas generation. In a laboratory model exploring temperature effects on anaerobic decomposition, Kasali and Senior noted that temperature increases from ambient temperatures (18.7 deg C) to 40 deg C greatly enhanced methanogenesis but when temperatures reached roughly 55 deg C, methanogenesis was inhibited (Kasali and Senior, 1989:40).

Most landfills operate in the mesophilic or thermophilic temperature range (Pacey, 1986:363), with landfill gas generation occurring in those temperature ranges as well (Chiampo and others, 1996:40). High temperatures within actual landfills can be achieved due to microbial activity despite low ambient temperatures of the prevailing climate (Rees, 1980:462). Most temperature changes are attributed to the anaerobic phase of degradation -- not because aerobic degradation is unable to produce significant amounts of heat as hypothesized by McBean, but because of the short-lived nature of the aerobic phase stemming from oxygen depletion (Rees, 1980:461-462).

Nutrients. Bacterial growth requires several essential nutrients (which nutrients depends on the bacterial species) to include carbon, hydrogen, oxygen, nitrogen, sodium, potassium, calcium, magnesium, phosphorous, and several trace metals (El-Fadel and others, 1996:314; Atlas and Bartha, 1993:236-240, McBean and others, 1995:75; Tchobanoglous, 1993:673). If the nutrients required by a particular bacterial species is not present, microbial cell synthesis and growth may be limited or cease altogether. Not only are the nutrients themselves required, but it may also be necessary for them to be in a

certain form or proportion for the bacterial species to utilize them. Moreover, if these required nutrients exceed particular levels, it may prove inhibitory to bacterial growth. However, usually the nutrients required for decomposition will be available from the waste within the landfill (Barlaz and others, 1990:575).

Oxygen and Other Inhibitors. Anaerobic bacteria can be either obligative or facultative in nature, obligative meaning they are unable to survive in the presence of oxygen and facultative meaning the anaerobes can grow with or without the presence of oxygen. Accordingly, oxygen is detrimental to those microbes which are obligate anaerobes such as methanogens. The presence of oxygen can cause complete cessation of a degradative step such as methanogenesis which depends on obligate anaerobes (El-Fadel and others, 1996:314).

Other inhibitors act much in the same way as oxygen as they disrupt the degradation processes by affecting the microbial populations responsible for the particular process. Examples of inhibitors include sulfate, heavy metals and numerous other toxic pollutants. Sulfate-rich environments have been documented as being inhibitory to methanogenesis because the sulfate-reducing bacteria outcompete the methanogens for electron donors such as H_2 and acetate, sulfate acting as the electron acceptor (Gurijala and Suflita, 1993:1180; Barlaz and Palmisano, 1996:43). Although some metals are required in trace amounts, the addition of heavy metals to a landfill in larger concentrations can limit microbial activity (Atlas and Bartha, 1993:237-238). With any of these inhibitors including any of the other possible toxic pollutants present in

significant concentrations, microbial growth and, subsequently, the degradation process can be retarded.

Model Approaches to Biodegradation

Realistic limits to the complexity of experimental studies of biodegradation, as well as their temporal and spatial limitations, limit the usefulness of such studies in ascertaining long-term behavior associated with decomposition (Moorhead and others, 1996:137). Various models have been constructed in hopes of simulating the underlying processes of degradation, with most utilizing mathematical or numerical approaches to modeling. By examining other models attempting to simulate biodegradation, one can witness the successes and failures of various authors in trying to represent such a complex ecosystem. Each of these modeling efforts is concerned with ascertaining what factors drive or influence decomposition and being able to simulate various scenarios or process behaviors over time.

Numerical Model of Gas Generation and Transport. El-Fadel utilized a numerical model in assessing the generation of landfill gas by incorporating biokinetic model equations to describe the degradation process (El-Fadel and others, 1997:87). Utilizing Monod based equations for modeling bacterial growth, first order rate equations for selected reactions such as hydrolysis, mass balancing, various physical processes such as gas flow within the landfill, and parameter values derived from the Mountain View Controlled Landfill Project in California, the model attempts to describe both the physical and biochemical processes in landfills (El-Fadel and others, 1996:131-134). The model focused on the fermentation and methanogenesis degradative steps and the corresponding

bacterial types. His results seem to correspond well with the data from the test landfill. From numerous simulations, the author hypothesized that the hydrolysis rate can become a limiting factor for gas generation and biokinetic parameters such as the half-saturation constant can have significant effects on degradation (El-Fadel and others, 1997:100-101).

Structured Modeling. J.D. Bryers proposed a "structured model" of anaerobic digestion which is a mathematical model employing matrix algebra to represent the components pertinent to the reaction scheme modeled (to include the reactants, intermediates, and products) and the stoichiometry involved in the reactions (Bryers, 1984:638-639). The model also incorporates reaction rate expressions and material balances to simulate anaerobic digestion. Structured modeling attempts to provide details of microbial composition, mixed-culture population dynamics, and multiple reaction mechanisms as a function of conditions in a biological system (Bryers, 1984:647). This effort focused on simulating various operating scenarios for an anaerobic digestor, and its results agree with two existing experimental studies of anaerobic digestion (Bryers, 1984: 638). The author emphasized defining the appropriate reaction scheme and its stoichiometry in order to accurately simulate microbial systems and processes (Bryers, 1984:647).

LEAGA-1 Model. Several authors from South Korea devised a model to simulate the production of methane by employing a model which combines a hydrological module with a biological module (Lee and others, 1993:225). The hydrological module attempts to incorporate the unsaturated flow of water within a landfill to represent the variation of moisture content. The biological module utilized Monod kinetics for the growth of

microbial biomass, Monod substrate depletion equations for production of intermediate substrates such as acetate and gas production, and a first order rate equation for hydrolysis. The model simulations were compared to laboratory experiments of degradation of landfill samples. The authors concluded that predicting the quantity of landfill gas produced was strongly dependent on biological parameters, and the hydrolysis rate constant played a significant role in predicting the percentage of gas (Lee and others, 1993:234).

Empirically Based Model. Findikakis employed a gas generation function based on field data to simulate gas production for a landfill (Findikakis and others, 1988:116). Although the author based the shape of the generation function on equations describing biochemical processes, the author admits such an empirical function does not explicitly incorporate variables such as moisture content and temperature which influence rate and composition of gas (Findikakis and others, 1988:122).

Other Models. Most other models documented in literature rely on mathematical algorithms incorporating Monod kinetics and first order rate reactions to address various microbial driven phenomenon in the degradation process (Rosso and others, 1995:610). J. Kaiser's (1996:25) modeling of composting and Young's (1995:74) model of anaerobic decomposition are typical. Some noteworthy approaches or conclusions include: Kaiser utilizing mass as the common unit in contrast to volumetric concentration in employing Monod kinetics (Kaiser, 1996:29-30); estimating kinetic parameters for degradation such as u_{max} or K by changing them jointly and simultaneously (Kaiser, 1996:30); Young's

model depicted an overshoot and collapse effect for methanogenic populations with access to large food reserves (Young, 1995:83).

Conclusions Derived from Model Research. By researching the various types of models, several conclusions can be reached regarding the representation of certain processes within biodegradation and variables considered to be most influential. It appears Monod kinetics is widely accepted in depicting microbial growth, and variations of Monod equations are employed in describing other processes such as substrate depletion. Biological parameters such as half-saturation constants can be quite influential in determining the state of progression for degradation. Stoichiometry plays a vital role in accurately representing the biochemical reactions occurring in decomposition. Finally, the influence the aforementioned environmental parameters can have on biodegradation may be significant, especially the parameters of moisture content, temperature, and pH.

Although the fundamental processes of biodegradation associated with landfill disposal have been aggressively studied by countless authors and modeled by a few others, it remains an extremely complex subject to understand and simulate. Modeling is typically limited to general descriptions of the overall process or intricate explanations or simulations of a particular reaction or bacterial phenomena associated with the process. Each of the aforementioned modeling efforts addressing biodegradation generally avoid viewing the process from a larger or "big picture" perspective in understanding the process. They sometimes fail to question whether the entities chosen for modeling are fundamental to the *overall* process. Moreover, significant interrelationships between entities in the degradation system and indirect influences on system behavior stemming

from changing entity conditions may be ignored or their effects suppressed by focusing on a particular aspect of the process. By choosing to concentrate on pieces of the system without addressing how all the pieces fit together in the system, some modeling approaches may fail to capture the true mechanisms responsible for the degradation process.

III. Methodology

System Dynamics Approach to Modeling

Biodegradation is a complex process involving countless interactions among numerous varied entities and parameters, from microorganisms to temperature to various substrates. It occurs in an ecosystem where change naturally occurs over time and the complexity of such change stems from the internal interactions of the system. To assess and model behavior over time of such a dynamic process and system, systems thinking in conjunction with a requisite mechanistic model prove ideal. System dynamics captures the feedback loops, multiple interactions, time sensitive behavior, non-linear interactions, and changes in the system over time associated with extremely complex systems such as the landfill bioreactor.

System dynamics reproduces system behavior mechanistically by identifying and simulating the underlying fundamental processes driving basic system behavior in contrast to other modeling approaches such as empirically based modeling which ignore the underlying processes (Moorhead and others, 1996:137). Moreover, since system dynamics allows one to simulate, it facilitates the study of the internal interactions of complex systems such as the landfill bioreactor system, the exploration of system behavior beyond the range of actual system observation, and better understanding of the implications of various parameters on the dynamic interrelationships of the system (Shelley, 1997).

For this thesis effort, the system dynamics approach will be utilized for the aforementioned reasons in modeling the fundamental processes of biodegradation which represent the landfill bioreactor ecosystem. Accordingly, the methodology for this thesis effort parallels the system dynamics modeling process. The basic steps of the system dynamics modeling process can be divided into four distinct phases: conceptualization, formulation, testing, implementation (Randers, 1996:119). It should be noted that the system dynamics process is an iterative one, requiring the modeler to repeat or modify any one of the modeling stages as necessary to ensure the model becomes a true mechanistic representation of the biodegradation process.

Conceptualization

To properly identify the system to be modeled, one must become familiar with the general system, processes, and interactions involved. To enhance familiarization with the system, one must also continually interact with appropriate experts in the field of study to ensure the requisite processes are addressed. Consulting with experts also assists in the establishment of appropriate boundaries for the model with regard to the model's intended purpose. Once familiarization with the problem area has occurred, one can focus on what causes a given development, specifically what is responsible for biodegradation within a landfill and the subsequent landfill gas behavior over time.

Literature Review. Initially, an extensive literature review is conducted in order to fully comprehend the entities and relationships driving behavior of the landfill bioreactor ecosystem. The primary focus is to gain a fundamental understanding of the natural progression of decomposition, determine the behavior of the microbial

populations involved in degradation, and not only which but also how environmental parameters affect biodegradation. The literature review includes consulting with available experts well-acquainted with the landfill ecosystem and microbial ecology. It is important that the literature review continue throughout the model building phase as questions dealing with plausible parameter values, system mechanisms, and system relationships arise. Once a general literature review is completed, a reference mode of system behavior or time development of interest can be described.

Reference Mode. A reference mode, or the expected behavior over the time period of interest, is derived by analyzing the thesis purpose, available historical data of the ecosystem, systems found in the literature, and expert input. It serves as an approximate picture of the expected output of the initial model (Randers, 1996:131). In this thesis effort, landfill gas generation serves as the metric for biodegradation; thus, it is also used as the time development of interest or reference mode for the modeling effort. As described in Chapter 2, the phases of landfill gas generation depict the progression of organic waste degradation within the landfill bioreactor. A majority of the literature concerned with landfill ecosystem behavior over time incorporate landfill gas as a metric of degradation (Tchobanoglous, 1993:385; McBean and others, 1995:72; Barlaz and Palmisano, 1996: 40; Pacey, 1986:52). Landfill gas generation from the four or five-phase approach for the progression of biodegradation can be utilized as the reference mode. See Figures 2 and 3 for possible depictions of the reference mode, one representing empirical data, the other theoretical in nature.

Influence Diagram. An influence diagram representing cause-and-effect relationships between the important entities which best represent the degradation process will be constructed. Using data gathered from the literature review, entities essential to the degradation process (real world mechanisms responsible for the reference mode) will be initially identified. Based upon this data and the reference mode, the influences between these entities will be defined and should generate feedback loops describing the basic mechanisms responsible for behavior of the degradation ecosystem. The level of aggregation and system boundary necessary to incorporate all relevant entities and influences are determined by the purpose of the thesis.

To illustrate the concept of an influence diagram, the following simple diagram is presented.

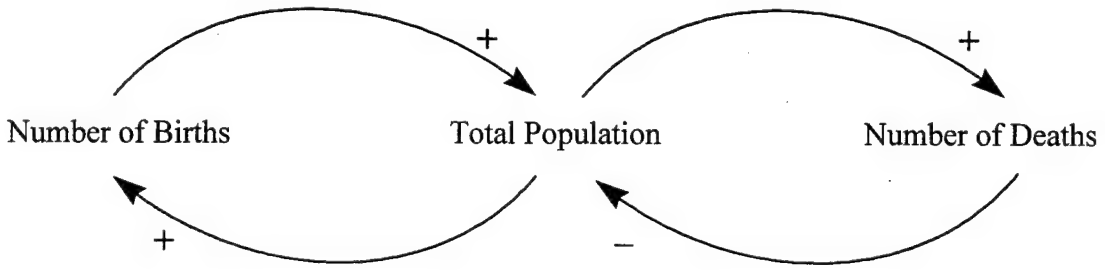


Figure 10. Simple Influence Diagram (after Roberts and others, 1983:47)

The arrows in the diagram represent some type of relationship between the entities. The "+" or "-" signs associated with the arrows depict a positive or negative relationship

respectively. A positive relationship assumes as one entity increases so does the entity associated with it while a negative one means as the entity increases, the entity associated with it decreases. A feedback loop is formed when the entities affect one another. Such loops can be positive or negative in nature. A positive loop results in behavioral changes being reinforced while a negative loop offers behavior which tends to dampen the initial response as the loop is traversed (goal seeking behavior).

The example diagram illustrates both types of causal loops. A positive loop defines the birth and population relationship (as the number of births increases so does the population and as the population increases so does the number of births) while the death and population relationship is a negative loop (as the population increases so does the number of deaths but as the number of deaths increase the population decreases). For a detailed explanation of causal loop and other system dynamics modeling notation, see *An Introduction to Systems Thinking* by High Performance Systems or *System Dynamics Modelling: A Practical Approach* by R.G. Coyle.

Creating an influence diagram is crucial to understanding how a system generates a behavior of interest. Not only does it denote the entities of the system, but it also depicts the nature of the relationships between such entities. The influence diagram allows the modeler to isolate critical causal factors driving the system behavior of interest. Moreover, it facilitates construction of the model by enhancing the modeler's understanding of how aspects of the model fit together. Prior to coding the influence diagram into STELLA, a software modeling package from High Performance Systems (STELLA II, 1994), the diagram will be presented to faculty to ensure that the diagram

incorporates the basic mechanisms responsible for ecosystem behavior and mechanistically describes the system's relationships. Due to relevant faculty input and additional literature review, the influence diagram may be altered accordingly to achieve the most accurate and relevant causal diagram.

Formulation

Once the system's mechanisms have been defined with an influence diagram, flow diagrams will be created. Flow diagrams explicitly identify which entities of the system from the influence diagram are levels and which are flows or rates. Consequently, flow diagrams are crucial in transforming the influence diagram into an actual model of the system by determining how the system entities need to be defined. Stocks of material and flows between stocks are utilized to represent the conversion of material from one phase to another. A stock or level is defined by the accumulation of the flows into and out of it with these flows defined by requisite equations representing the nature of the flow. For example, using the simple influence diagram of Figure 10, a flow diagram is created as depicted in Figure 11.

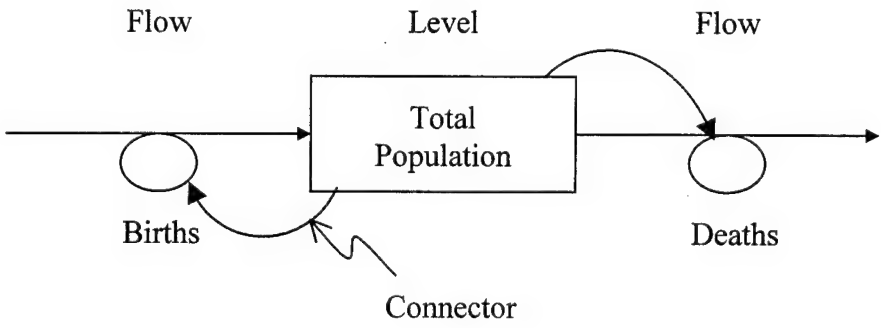


Figure 11. Simple Flow Diagram

Both the number of births and deaths define the total population as denoted in the influence diagram, but the flow diagram clarifies the system and its relationships even further. The flow diagram identifies the population as a level and the number of births and deaths as flows affecting the level of population. The level accumulates or declines based on the flows in and out of it. The "connectors" between the population and birth/death flows represent the effects total population has on the number of births and deaths as denoted in the influence diagram (Figure 10). The flows into and out of the total population entity and the connectors combine to depict the loops of the influence diagram. STELLA is essentially a software package which allows for such flow diagram construction in the model building process.

The system dynamics model is constructed by coding the flow diagrams into the STELLA computer modeling software which creates the corresponding system of simultaneous differential equations and solves them using traditional numerical integration techniques. Each sector of the model postulates a detailed structure depicting the flow diagrams with appropriate levels and rates selected from gathered data. Equations defining such levels and rates, as well as any parameter values, will be formulated from literature and faculty input. Assumptions regarding any model formulations, parameter values, or relationships are documented in Appendix B.

Testing

Testing the Dynamic Hypothesis. Initial model runs will be conducted to determine whether the basic mechanisms of the model reflect the reference mode. If the

model does not reflect the reference mode, additional review is required to determine if it includes all of the essential variables and mechanisms responsible for system behavior, if the assumed relationships are reasonable, and if the parameter values are plausible. Additional review may also lead to questioning the appropriateness or accuracy of the reference mode itself. During testing, the model will be modified accordingly, consulting with faculty and performing additional literature review to correct any discrepancies. Although it is impossible to prove the absolute correctness of any model in representing reality, one can build confidence in a system dynamics model by comparing it to reality through validation testing (Legasto Jr. and others, 1980:211). There are numerous confidence tests which can be applied to a model, but one must determine the appropriate ones given the nature of the model.

Structure Verification Test. For this test, the structure of the model is compared directly to the structure of the system the model represents. It may include verification by persons knowledgeable in the area modeled or comparing model assumptions to relevant literature. To pass the test, the structure of the model should not contradict knowledge about the real system; however, it does not mean that every detail known about the system must be incorporated into the model to pass the test.

Parameter Verification Test. Model parameters (constants) should be compared to real observations when possible to ensure conceptual and numerical adherence. If such comparison is not possible, experts and literature are consulted to ascertain the plausibility of parameter values. Moreover, behavioral testing can help determine the validity of parameter values by identifying unreasonable behavior for the

system when certain values are utilized in the model. Those constants which could change over the long term should be represented as a variable to reflect their changing status over time.

Extreme Conditions Test. The consequences of extreme conditions for the model should be explored by adjusting the levels on which rate equations in the model depend toward extreme levels. For example, if an input to a process is set at zero, then output should be zero. By inducing extreme conditions, confidence in the model is built by witnessing plausible behavior for a wide range of plausible conditions.

Boundary-Adequacy Test. This test determines whether the model includes all relevant structure given the model's purpose. Is the model's level of aggregation appropriate. To conduct the test, a hypothesis which addresses a change to the model structure is developed and then incorporated to resolve the importance of the hypothesized structure change. If there is no significant change in the resultant behavior, then the basic model structure does not need to add the hypothesized structure. This test also incorporates behavior testing by analyzing behavior with and without additional structure.

Behavior Reproduction Test. Behavior reproduction testing seeks to compare how well model generated behavior simulates realistic behavior. The key word is behavior; predicting *exact* future values of a real system or *replicating values* of past data is not an appropriate basis for evaluating a system dynamics model (Legasto Jr. and others, 1980:218). A particularly appropriate test in this family of tests is the relative phase test which centers on the phase relationships between variables. The relative phase

test focuses on testing whether the relative timing of variables of the model matches the relative timing of those variables in the real world. In other words, do the relevant variables of the model follow the same timing sequence as that found in the real world system? If one can show a particular behavior resulting from model simulation is a necessary consequence of the model structure, then confidence is built. Moreover, it must be emphasized that inputs from outside the established model boundary should not drive the general pattern of behavior.

Behavior Anomaly Test. If one discovers model behavior contradicting real or intuitive behavior, the behavior can be considered anomalous. Tracing the behavior can often lead to weaknesses in the model assumptions or insights into real system potential behavior. This test can also be used to defend a particular assumption by illustrating anomalous behavior if the assumption is altered.

Sensitivity Testing. Sensitivity testing identifies sensitivity in model output to changing parameter values, thereby offering insight into the attributes of the model most sensitive to perturbations or manipulations of the model. By changing the values, one can analyze the impact of the parameters on behavior. Although, most plausible changes to parameters result in little change to behavior, identifying a sensitive parameter does not necessarily invalidate the model.

Implementation

Presentation of Findings. Results from model runs will be consolidated and translated into a useable form to facilitate examination of the model output. Assumptions for the model will be reemphasized to ensure the context of the model's scope and

structure is well understood. The focus of the presentation will center on determining whether the system dynamics approach achieved the thesis purpose and offering insight into biodegradation while addressing the influence of environmental factors.

IV. Results And Discussion

Conceptualization of Biodegradation/Landfill Bioreactor System

Employing the initial step of system dynamics methodology, conceptualization of the biodegradation processes and landfill bioreactor system, results in the development of the reference mode represented in Figure 12. Although Figures 2 and 3 represent adequate reference modes for the model, they both include atmospheric nitrogen gas (approximately 79% of ambient air, by mass), thereby suppressing the apparent relative contribution of microbially-generated hydrogen gas within the landfill. Figure 12 is based on the reference modes of Figures 2 and 3, correcting the relative concentration of hydrogen gas in the absence of atmospheric nitrogen. Therefore, the curves representing each type of landfill gas generated in Figure 12 are smoothed representations of behavior based on the graphs of Figures 2 and 3. The Roman numerals listed at the top of the graph represent phases of the five-phase approach while the titles for each phase are from the four-phase approach.

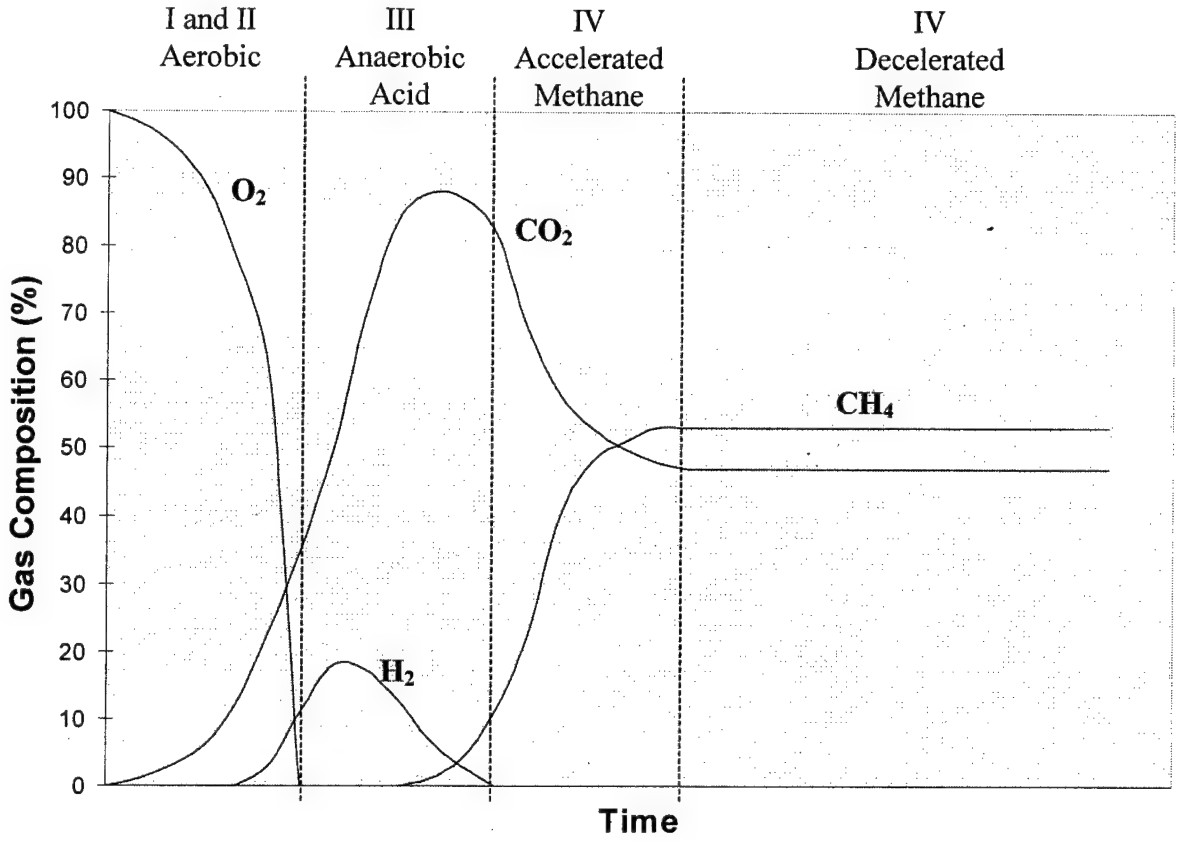


Figure 12. Theoretical Reference Mode from Literature Sources

Ultimately, Figure 12 is based on empirical data by virtue of Figures 2 and 3 being founded on field and laboratory testing, but Figure 12 itself is not a graph of exact measurements from field or laboratory data. The time frames associated with the x-axis of Figure 12 for each phase of degradation are provided in Table 5 to illustrate the *typical* time periods associated with the degradation process. These time periods are approximations derived from literature based on certain initial landfill conditions as noted in the table. Actual time frames will differ depending on varying landfill and environmental conditions.

Table 5. Typical Time Periods Associated with Biodegradation

Phase	Time Period (days)	Remarks
I and II Aerobic	3 to 10	Dependent on availability of additional oxygen and refuse moisture content.
III Anaerobic Acid	10 to 50	Saturated conditions result in 70 % CO_2 being produced in roughly 11 days
IV Accelerated Methane	To reach steady state methane production --- 90 +	Approximately 90 days for wet refuse, much longer for dryer refuse.
IV Decelerated Methane	From initial steady state to decline in methane production --- 90 days to years	Dependent on refuse organic material availability.

From the reference mode and additional literature review, the influence diagram depicting the cause-and-effect relationships of the landfill bioreactor is constructed. The final influence diagram splits the biodegradation process into two stages: aerobic and anaerobic (See Figure 13 for the influence diagram.).

Figure 13. Influence Diagram

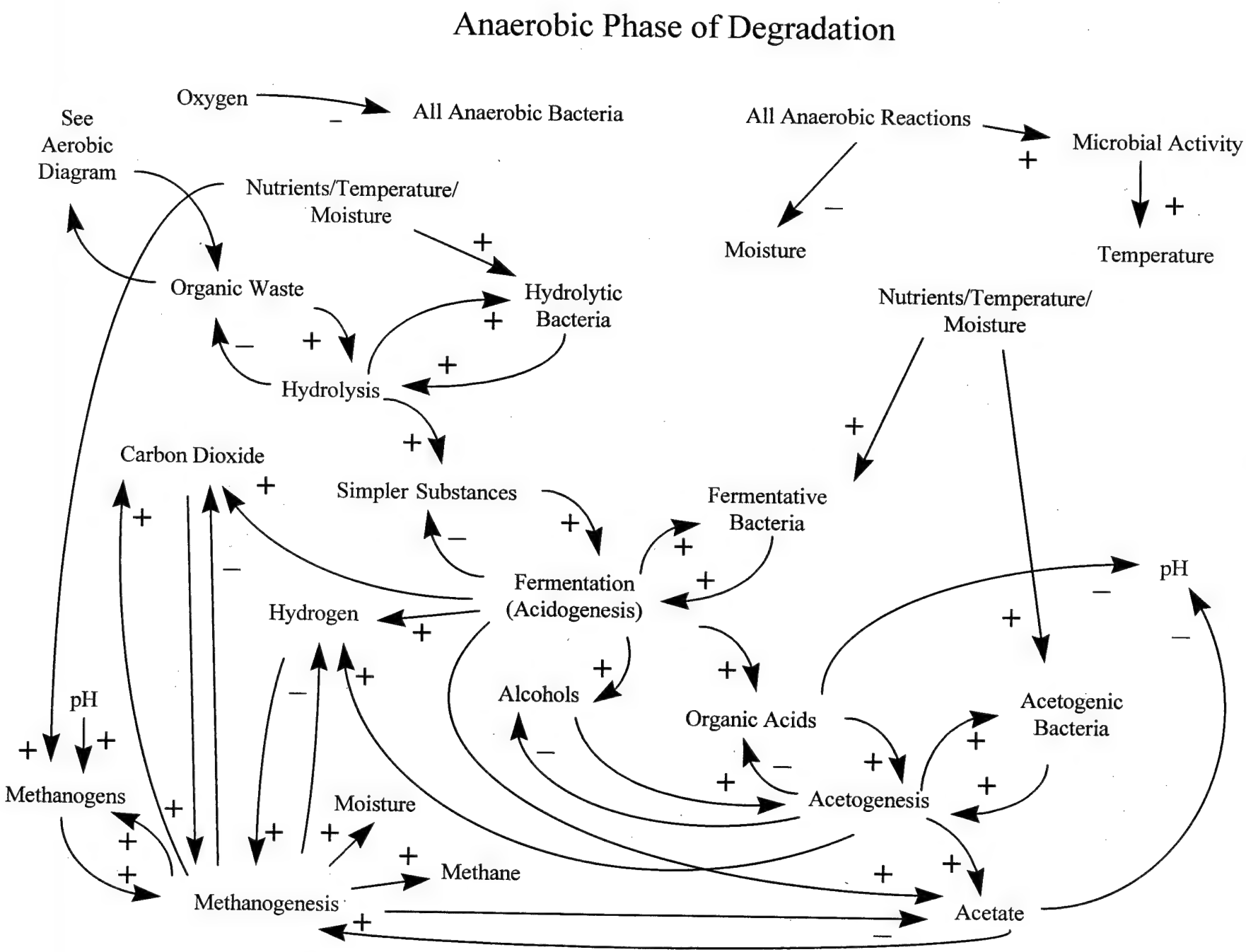


Figure 13. Influence Diagram

As the diagram illustrates, there is a natural progression of events with microbial populations influencing each degradative step. This natural progression of events can be witnessed in the reference mode itself as each degradative step produces, ceases to produce, or consumes a type of landfill gas. Environmental factors such as moisture content also impact each step by influencing the microbial populations which in turn drive the flow of the process.

The feedback loops for the system are predominantly located between the bacteria and each degradative step and the bacteria and their particular substrate. These feedback loops primarily define the cause-and-effect behavior for the landfill bioreactor system. When viewing the influence diagram, it is important to note the type of relationship between entities as well as the feedback loops created. A positive feedback defines the relationship between bacteria and degradative process while a negative feedback exists between bacteria and substrate. Noting which type of feedback predominates allows one to visualize what type of behavior results from the relationship, whether it is a self-reinforcing or limiting type of behavior. The effects of environmental parameters on the overall biodegradation system stem from their influence upon the bacteria themselves.

Formulation/Model Construction

Using the influence diagram as a guide to the relationships and mechanisms found in the system, a flow diagram is constructed. The overall flow diagram for the system can basically be broken down into two separate and distinct flows. One major flow represents the progression of degradation (delineated from the influence diagram of Figure 13) from the aerobic phase to methanogenesis as discussed in Chapter 2. Another major flow

depicts the growth and decline of each of the various bacterial groups involved in the decomposition process.

To simply illustrate each generic type of flow and their relationship between each other derived from the influence diagram, Figure 14 is presented. The entire flow diagram for the system is represented by the model structure constructed with STELLA software. See Appendix B.

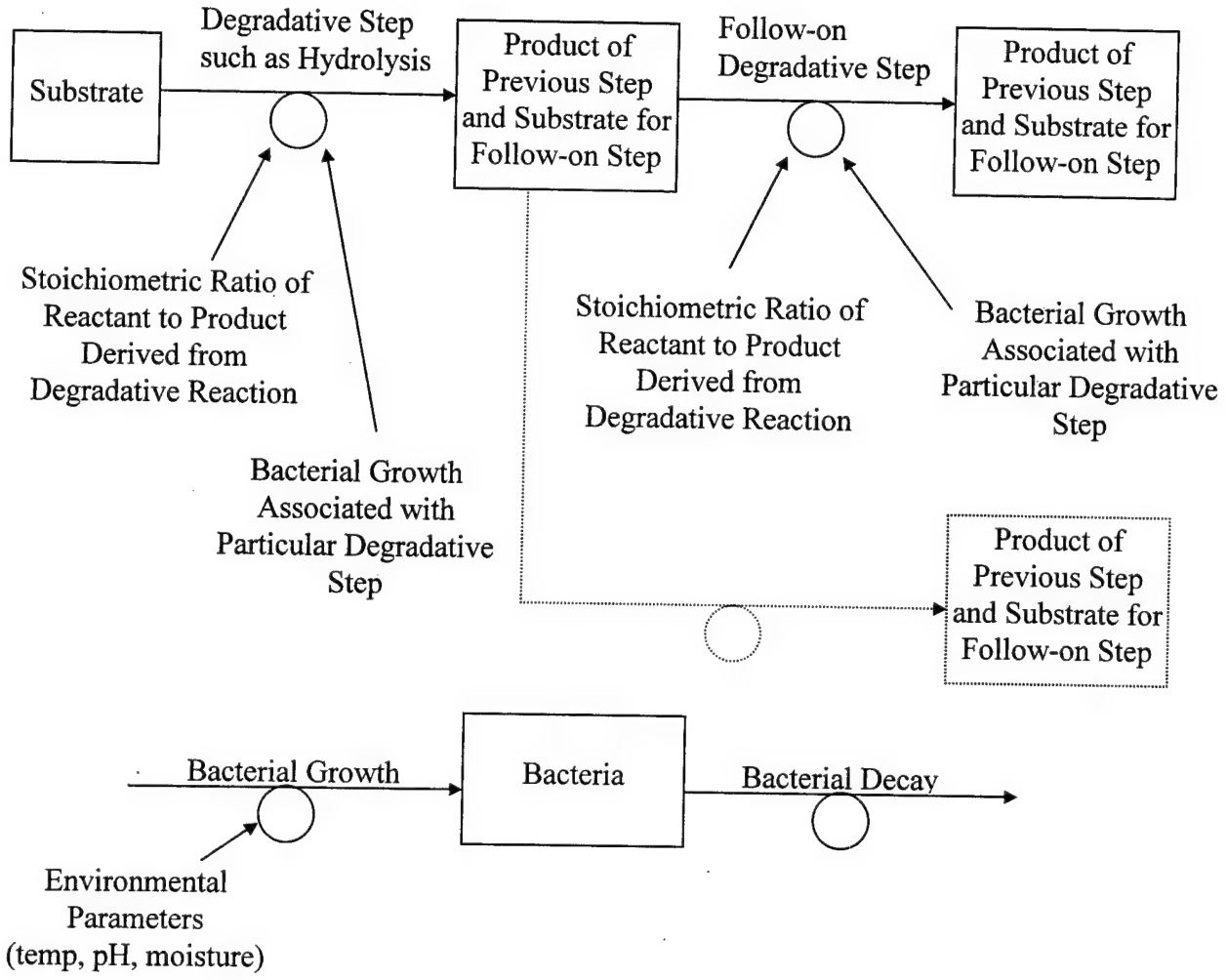


Figure 14. Generic Flow Diagrams of the Model

Figure 14 demonstrates how the progression of degradation and bacterial groups are represented through a flow diagram, but more importantly, how biodegradation is interrelated to the presence and growth of bacteria. The dotted line represents the possibility of more than one product resulting from a particular degradative step. Note the importance stoichiometry plays in determining the proportion of product based on the degradative reaction. The influence of environmental parameters centers on bacterial growth. What is important to gain from the flow diagrams presented in Appendix B and Figure 14 is an understanding of which system entities are levels or rates and of the nature of the relationship between the entities.

By viewing the overall flow diagram of Appendix B and Figure 14, it is apparent that the relationship between substrate depletion or conversion and bacteria is indispensable to the functioning of the system. The products produced, the rate at which they are produced, and the subsequent progression of degradation (or whether a degradative step occurs at all) stems from this relationship. Defining this relationship is critical in providing a mechanistic representation of the landfill bioreactor system. The model equations utilized to define the numerous and different relationships between the various bacteria and substrates of the system are contained in Appendix C.

In formulating an equation to express the relationship driving the conversion of material, the following substrate depletion equation derived from Monod kinetics is employed (Metcalf and Eddy, 1991:371; Gaudy and Gaudy, 1980:236-240).

r_g or $dX/dt = -Yr_{su}$ where r_g = rate of bacterial growth (mass/unit vol x time)

Y = maximum yield coefficient (mass of cells formed to the mass of substrate consumed

r_{su} = substrate utilization rate (mass/unit vol x time)

Thus, r_{su} or dS/dt becomes

$$r_{su} \text{ or } dS/dt = -\frac{u_m XS}{Y(K_S + S)}$$

This equation provides the link between the degradative step and the bacteria responsible for each step since it is derived from Monod bacterial growth equations. Although the substrate depletion equation and the Monod equations for bacterial growth are normally based on concentration, the mass basis was utilized to simplify the model by assuming the same initial volume of waste for all components of the model. The depleted substrate material flow is also governed by stoichiometric considerations. Stoichiometric ratios delineating the proportion of materials as they are converted for the next phase of degradation are derived from the stoichiometric equations for each phase (see Chapter 2).

The bacterial populations themselves are in accordance with the degradative steps as discussed in Chapter 2 with Monod kinetics governing their growth and a first order decay rate their "death." When appropriate (methanogens) the dual substrate formula is used to reflect the possibility of either of two substrates becoming limiting in nature. The parameter values for the Monod equation and cell yields reflect the higher efficiencies of

aerobes as compared to anaerobic bacteria, thus their chosen parameter values ensure faster and higher growth for the aerobes. Initial values for bacteria also reflect the difference in initial mass of bacteria prior to the start of decomposition with the aerobes at a greater mass than the anaerobic bacteria (anaerobic bacteria are present initially but not growing).

Although the parameter values employed by the model reflect the general differences in efficiencies between aerobic and anaerobic bacteria, the values lack the definitive nature of values derived from specific laboratory or field testing. The parameter values are based on available literature values (see Parameter Verification section), but these literature values represent specific laboratory or field conditions. Values chosen for the model attempt to address the efficiency differences of the bacterial system while pursuing the realistic values from literature sources. However, the difficulty in ascertaining accurate values for the model (especially given the mass basis of the model) remains a limitation for the model and one of the significant areas that needs to be addressed in the future. See Appendix A for detailed assumptions regarding parameter and initial values for the various types of bacteria.

The environmental parameters, moisture content, pH, and temperature, begin at 40% by weight, slightly above neutral (roughly 7.8), and 20 deg C, respectively. For purposes of this model, external environmental interaction is not considered to occur within the boundaries of the model. Environmental parameters such as temperature and moisture in actual landfills are often affected by interactions with the environment. Both moisture content and temperature affect each bacterial group equally, while pH only

influences the methanogens. Moisture content is affected only by the consumption and production of moisture during the degradative process.

The effect of moisture on the growth rate of bacteria is represented through a moisture factor represented with a graphical function which ensures that as moisture content increases bacterial growth increases, but marginal growth slows as saturation is approached. See Figure 15 for an approximation of the graphical function employed in the model. A moisture content roughly between 40 and 50 percent is considered a fairly typical condition for a landfill in this model. If moisture content exceeds this level, bacterial growth accelerates albeit at a slower marginal rate as saturation is approached.

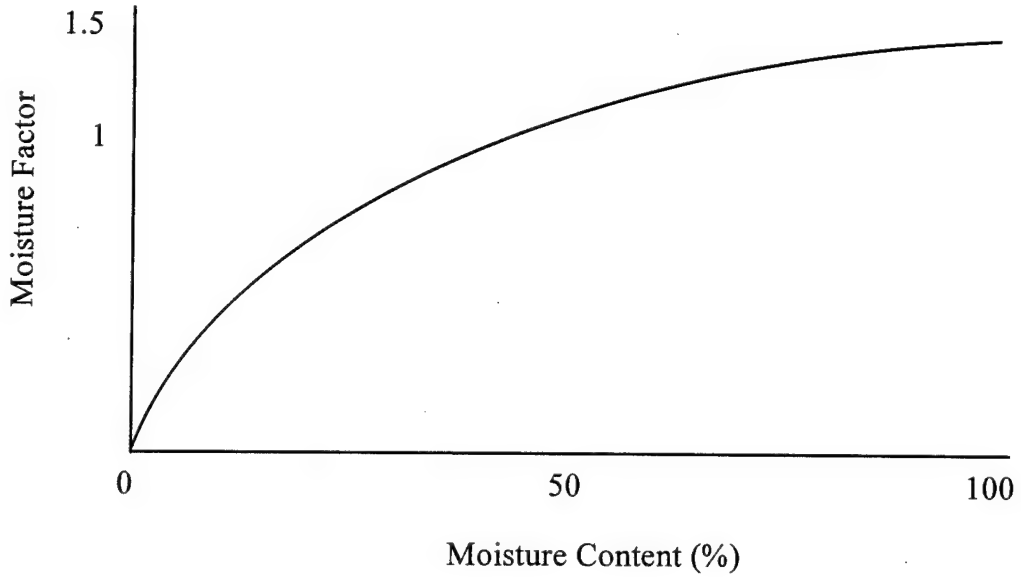


Figure 15. Graphical Function of Moisture Factor

pH is dependent on the acid production of the system. Acid accumulation for the model is represented by the combined stocks of organic acids and acetate. As acids increase, pH decreases until the acids are consumed which allows pH to rise. The pH factor is a graphical function based on the optimal range of pH for methanogenesis discussed in Chapter 2. An illustration of the graphical function and an appropriate discussion of the pH factor follow in the Structure Verification segment of the Testing section of this chapter. If pH is within the optimal range, methanogenesis is not inhibited. It is only inhibited if the optimal range is exceeded on either side.

Temperature changes are based on microbial activity. Microbial activity stems from bacterial growth rate. As microbial activity increases so does temperature. Then as temperature increases, bacterial growth rate climbs (within the optimal temperature range) which in turn affects microbial activity. Optimum temperature ranges assume that mesophilic and thermophilic ranges up to 50 deg C do not inhibit bacterial growth. Temperatures above 50 deg C become severely inhibitory to bacterial growth rapidly.

Testing

With the model constructed, numerous simulations were conducted for comparison to the reference mode, for validation testing, and for sensitivity analysis. Initially, the model's parameters were set to reflect the general assumptions associated with degradation and the values listed in Appendix A. The model, if accurate in accordance with its assumptions, should present behavior similar to the reference mode, which represents a realistic picture of landfill gas generation driven by the fundamental processes of biodegradation. Figure 16 represents model output with the initial

conditions and assumptions for the landfill bioreactor system. This model output (and associated parameter values) will form the basis for all validation and sensitivity testing.

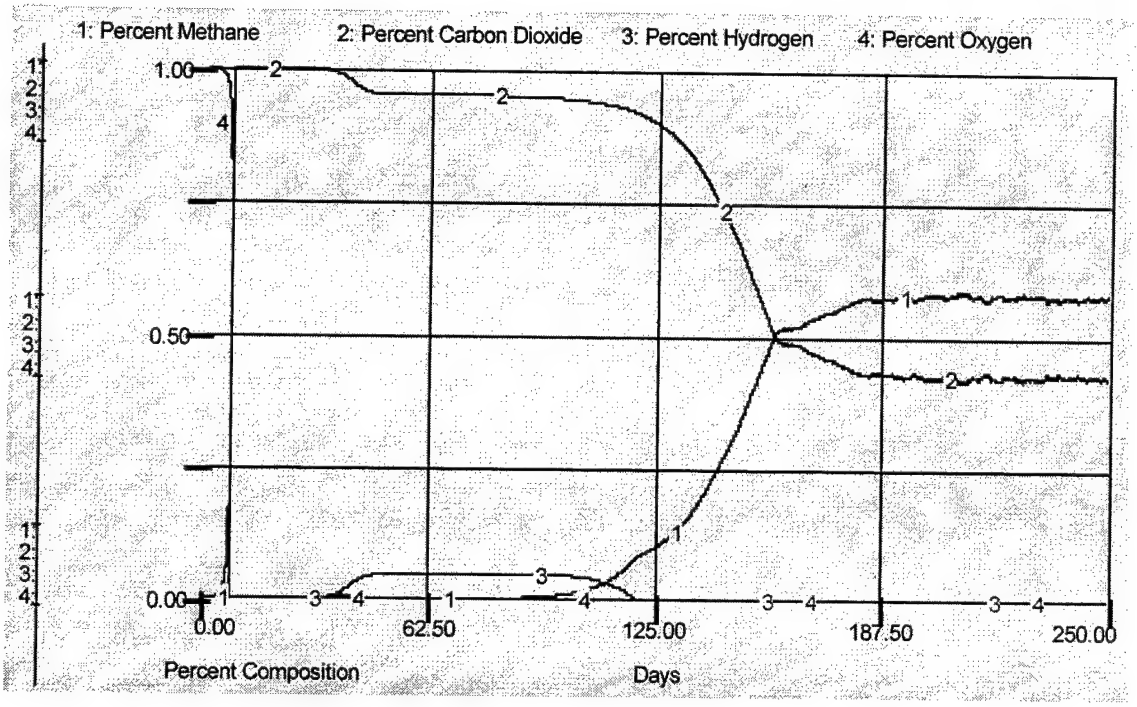


Figure 16. Basic Output of Model

As illustrated in Figure 16, the model reasonably simulates the fundamental landfill gas generation behavior associated with biodegradation. Oxygen is depleted fairly quickly, hydrogen gas is produced, and methane and carbon dioxide eventually reach an equilibrium roughly splitting the composition of the landfill gas generated. Comparing Figure 16 to the reference mode, Figure 12, one can conclude the basic mechanisms of the constructed model create the general behavior and progression of the reference mode. It appears the overall dynamic hypothesis of biodegradation has been successfully modeled; however, confidence in the model must be built before the model

can be considered successful in fulfilling its intended purpose of representing the fundamental processes of biodegradation associated with landfill disposal of waste.

Structure Verification. To verify the structure of the model, it must be compared to the structure of the real world. Before model construction began, an influence diagram was created as depicted by Figure 13. The influence diagram was based on relevant literature as well as a reference mode derived from empirical studies. From the influence diagram, the structure of the model was built; thus, the structure is founded on biodegradation and microbial principles from extensive literature review. For example, to depict microbial growth and its connection to substrate depletion, Monod kinetics were used, the most widely used microbial growth model (El-Fadel and others, 1997:245). Another example is the environmental parameters chosen for the model, especially those modeled as variables (temperature, pH, and moisture content). El-Fadel and others in a recent critical review of gas generation, confirm that these parameters have the highest potential as inhibitors to the degradation process (El-Fadel and others, 1997:240). Table 6 typifies their research into these parameters.

Table 6. Effects of Variables Influencing Gas Generation in Landfills (after El-Fadel and others, 1997:240)

Variable	Gas Inhibition Potential		
	Low	**Medium**	**High**
Waste Composition		X	
Temperature			X
pH			X
Nutrients	X		
Oxygen			X
Sulfate		X	
Toxics		X	

Not only have these influential parameters been drawn from literature review, but the shape of the curves delineating the influence of these parameters in the model also follow the optimal curves explaining parameter effects found in literature. For example, Figure 17 displays an approximation of the "curve" employed by the model to represent pH effects.

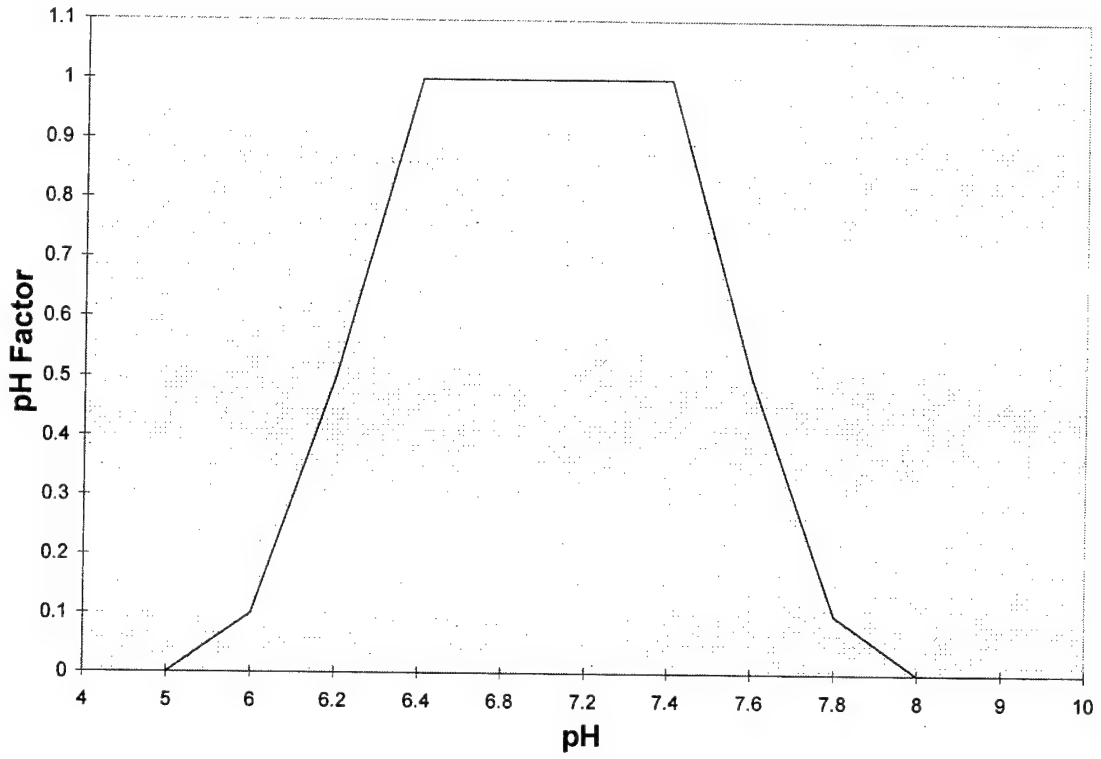


Figure 17. Model Curve for pH Effects on Methanogenesis

As denoted by the graph, the optimal pH for methanogenesis ranges from roughly 6.4 to 7.4, corresponding to a pH factor of "1" which allows methanogen growth to continue uninhibited in this range. Outside this optimal range, pH becomes inhibitory to methanogen growth.

Clearly, the degradation process is extremely complex, and many variations exist regarding the overall progression of the process, as well as the intricate reactions and influence of various environmental factors. However, given the model's purpose in pursuing the *fundamental* processes associated with biodegradation, the structure of the model, given its basic mechanisms and influences, compares favorably to the processes of

the real world landfill bioreactor in undergoing waste decomposition. Yet, literature confirmation alone cannot suffice in building confidence in the structure of the model. To demonstrate confidence in the structure of the model, its mechanisms, influences, and material flows, it should also be critiqued by those persons highly knowledgeable about the real system. For this thesis, the structure was reviewed by faculty members familiar with both landfill mechanisms and microbiological phenomenon.

Both review of the structure during model testing and faculty critiquing revealed a weakness in the model concerning substrate availability. Even under ideal conditions, bacteria will not have the entire mass of substrate available immediately nor will bacteria be able to attack anything but the surface of the substrate. Currently, the model assumes that if substrate is available it is wholly consumed by the bacteria. With this assumption, it becomes necessary to make the initial amount of organic waste extremely large to preclude its depletion in an unreasonable short period of time. Figure 18 demonstrates the substrate availability weakness using hydrolytic bacteria and its substrate of organic waste as an example. The other bacterial relationships are similar in nature.

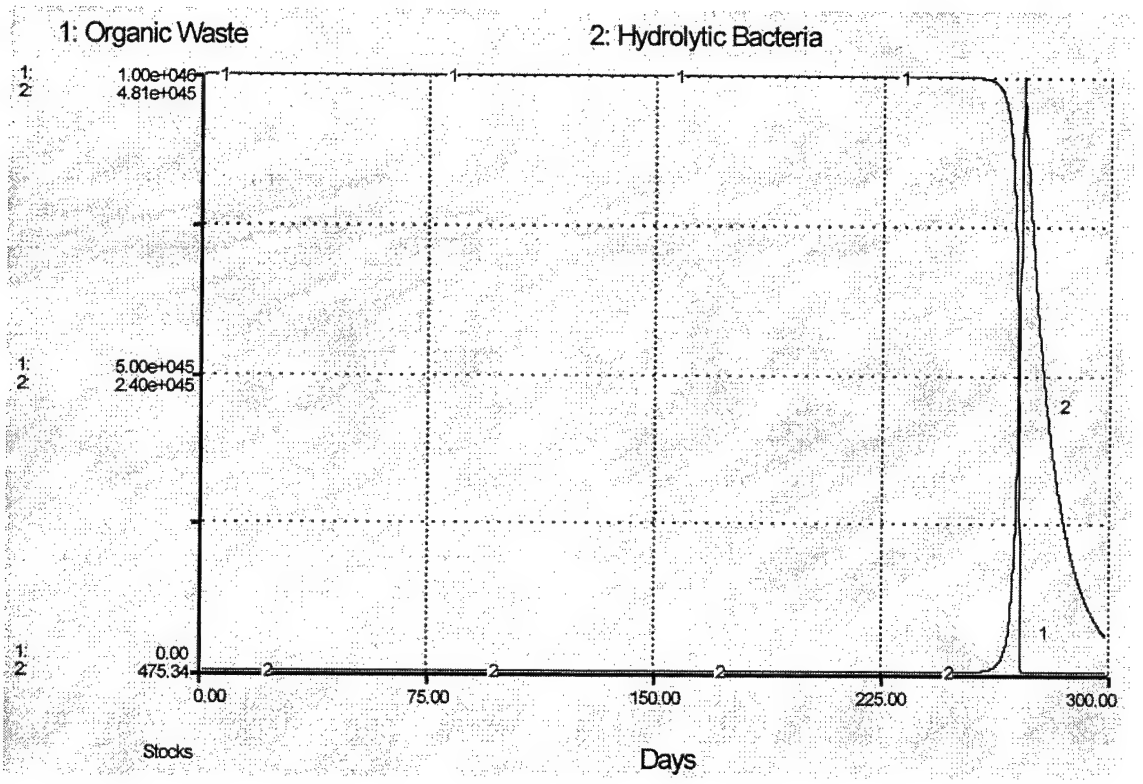


Figure 18. Relationship Between Bacteria and Substrate

The graph is presented to capture the relationship between bacteria and substrate towards the end of the simulation. Depletion and growth occur throughout the simulation, but they are masked in earlier time frames because of the output scaling (note the large values of initial organic waste and bacteria generated). Figure 18 is shown to illustrate how the bacteria population continues to climb even as the substrate is depleting, beginning its decline only when the substrate is *completely* gone. However, in reality the entire mass of substrate will not be available to the bacteria and more reasonable ratios of initial substrate to bacteria can be used for the model. This weakness of the model can also be illustrated in the growth rates shown in Figure 19. Traces 1

through 5 represent aerobic, acetogen, fermentative bacteria, hydrolytic bacteria, and methanogen growth rates, respectively.

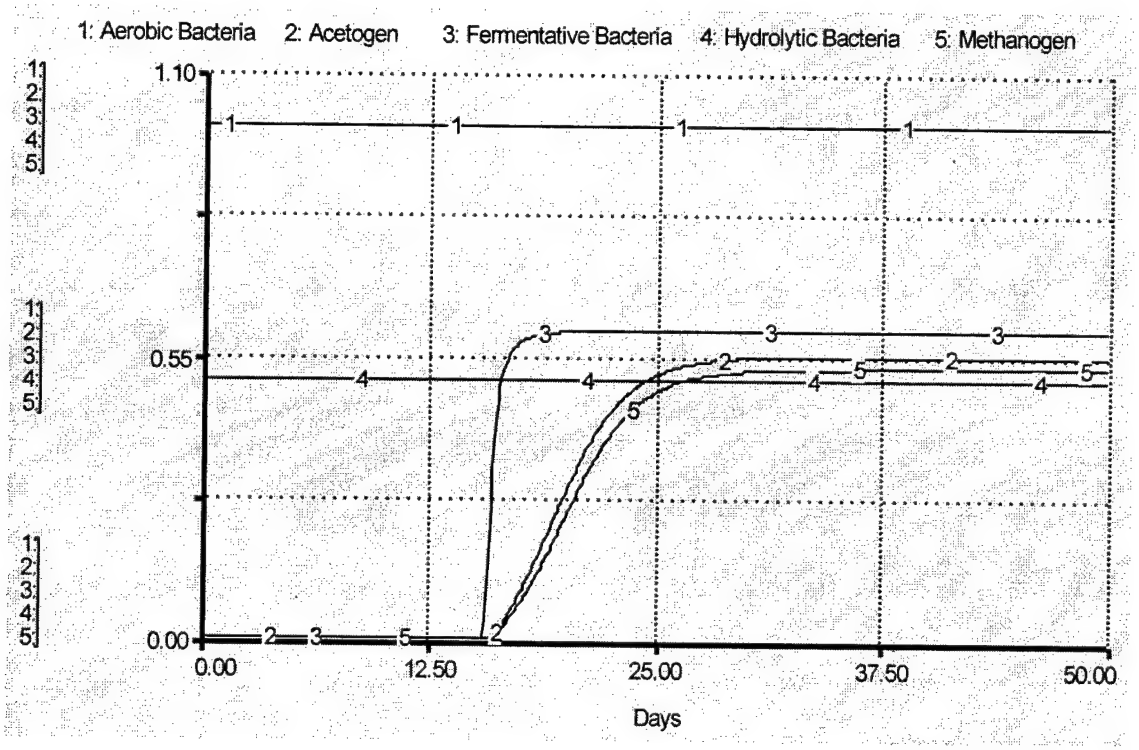


Figure 19. Bacterial Growth Rates

From Figure 19, it is evident the growth rates associated with aerobes and hydrolytic bacteria do not climb to their maximum growth rates as Monod kinetics dictate. Instead, their growth rates are already at their maximum value. In contrast to the other bacteria, the aerobes and hydrolytic bacteria of the model already have plenty of substrate available for growth, so much in fact that they *begin* growth at the maximum rate. Obviously, there will be an adjustment time for bacteria within their surroundings, and bacteria will be unable to attack the entire mass of substrate as discussed earlier.

Thus, Figure 19 further confirms that a mechanism addressing substrate availability is warranted for the structure of the model.

Another weakness regarding the structure of the model stems from the syntrophic relationship between acetogens and methanogens. Acetogens rely on methanogens to remove hydrogen for continued growth and methanogens on acetogens for the production of certain substrates, so if methanogens fail to remove the hydrogen, then hydrogen accumulation should become inhibitory to the acetogens. The result should be a halt in hydrogen production as acetogens wait for the requisite number of methanogens to do their job. Figure 20 depicts such a scenario where it is simulated that methanogenesis is not consuming hydrogen.

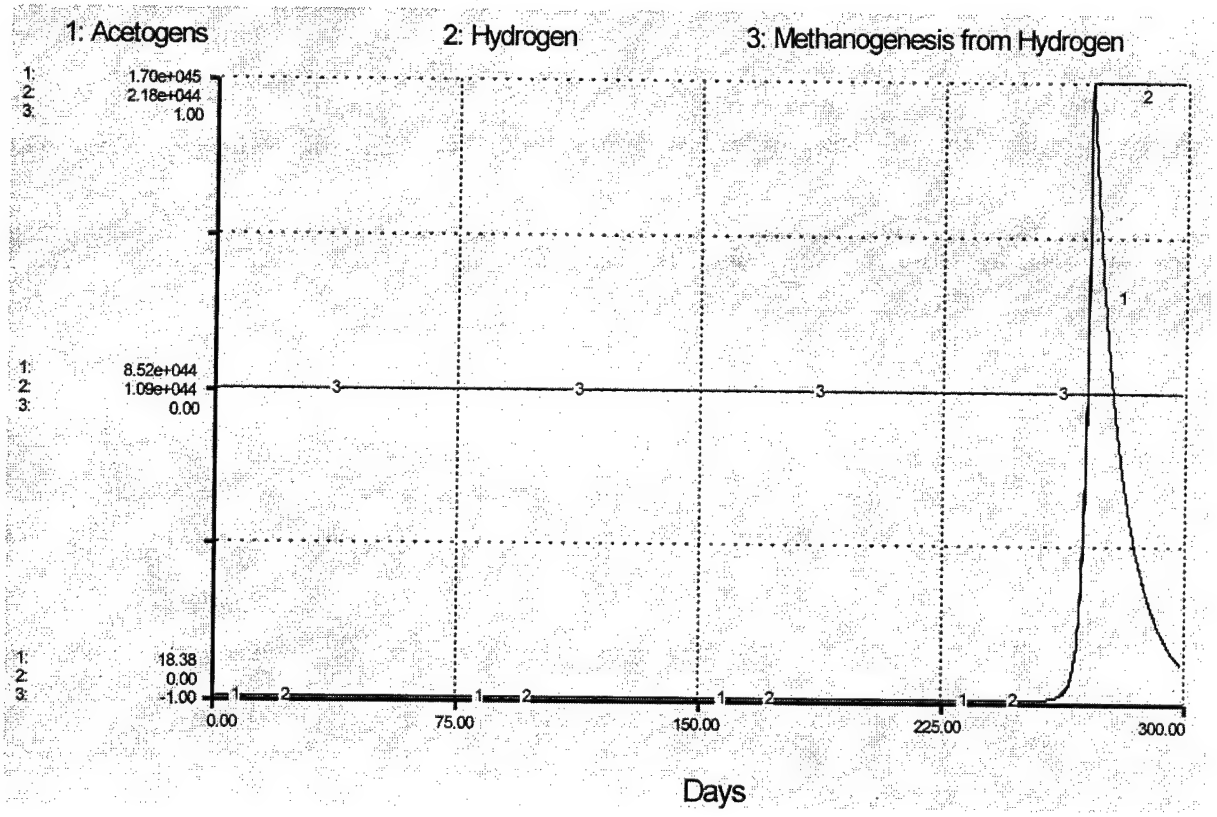


Figure 20. Syntrophic Relationship Between Acetogens and Methanogens

As Figure 20 illustrates, even though hydrogen is not being consumed by the methanogens, hydrogen production and acetogen growth are not altered. The present model certainly simulates both hydrogen production and consumption by the requisite bacterial groups; it merely fails to completely address the syntrophic relationship between acetogens and methanogens under less than optimal conditions for either bacteria.

Parameter Verification. Model parameters are compared to observations of the real world. These parameters must parallel real world parameters conceptually and numerically to build confidence in the model. For this thesis, both experimental laboratory studies and field testing results from literature were used in determining plausible parameter values.

In justifying parameters conceptually, the parameters were compared to elements of the system structure based on literature review and appear to capture basic elements of the fundamental processes of biodegradation. For example, a majority of the parameters in the model stem from bacterial growth, an area extensively modeled utilizing Monod kinetics. The parameters, u_{max} (maximum specific growth rate), Y (yield coefficient) and K (half-saturation constant), are derived from Monod kinetics literature and have been proven to correlate to the real world phenomenon of bacterial growth. The environmental parameters of temperature, pH, and moisture content are considered variables dependent on other entities of the model and also match critical elements of biodegradation. The stoichiometric ratio constants, conceptually (and numerically), were derived directly from the biochemical principles and equations which established the chain of reactions driving degradation as discussed in Chapter 2.

Numerically, parameter values can be compared to literature-based values, where they exist. For parameter values not found in literature, experts were consulted to at least ensure the parameter is conceptually accurate and numerically plausible. Unfortunately, for several entities such as the half saturation constant in the model, numeric validation proved extremely difficult since the thesis effort does not focus on one particular laboratory or field experiment. With parameter values often depending on the conditions present in the system, the validation of such parameters centers on plausibility when utilizing literature based values for comparison. Table 7 lists the parameter values employed in the model and the values found in literature. Assumptions concerning the parameter values are listed in Appendix A.

Table 7. List of Model Parameter Values

Model Entity	**Model Value**	**Literature Value (Reference)**	**Remarks**
Aerobe u_{max} (d^{-1})	1.0	No specific value found.	The value is greater than all anaerobic bacteria due to known greater efficiency of aerobes and aerobic degradation compared to anaerobic bacteria and processes.
Aerobe Y	0.6	0.4 to 0.6 (Gaudy and Gaudy, 1980:239-240)	Highest Y to reflect greatest efficiency in converting substrate to energy.
Aerobe K (mg)	50	No specific value found.	The lowest K value of the bacterial groups involved demonstrates the efficiency of aerobes. Since no literature value was found for comparison, the value is chosen to reflect the efficiency concept. (Conceptually, they reach their maximum growth rate first.)

Hydrolytic Bacteria u_{max} (d^{-1})	0.5	No specific value found.	No specific value for hydrolytic bacteria was found, but value based on efficiency concept and other anaerobic values found.
Hydrolytic Bacteria Y	0.5	0.4 to 0.6 (Gaudy and Gaudy, 1980:239-240)	Y value between lowest anaerobic stage and aerobic stage to reflect efficiency of converting substrate to energy below that of aerobes but above other anaerobic species.
Hydrolytic Bacteria K (mg)	250	No specific value found.	No specific value for hydrolytic bacteria was found, but value based on efficiency concept and other anaerobic values found. Model value from mass basis while literature value in concentration (mg/L).
Fermentative Bacteria u_{max} (d^{-1})	0.6	1.7 to 30 (El-Fadel and others, 1997:247) Critical review based on numerous studies.	Rates vary depending on composition of substrate and experiment. Lower value used to emphasize field conditions vice optimal laboratory conditions.
Fermentative Bacteria Y	0.5	0.4 to 0.6 (Gaudy and Gaudy, 1980:239-240)	Y value between lowest anaerobic stage and aerobic stage to reflect efficiency of converting substrate to energy below that of aerobes but above other anaerobic species.
Fermentative Bacteria K (mg)	500	23 to 37,000 mg/l	Model value from mass basis while literature value in concentration (mg/L).
Acetogen u_{max} (d^{-1})	.55	1.7 to 30 (El-Fadel and others, 1997:247) Critical review based on numerous studies.	Rates vary depending on composition of substrate and experiment. Lower value used to emphasize field conditions vice optimal laboratory conditions.
Acetogen Y	0.4	0.4 to 0.6 (Gaudy and Gaudy, 1980:239-240)	Y value reflects lowest efficiency of converting substrate to energy.
Acetogen K (mg)	750	23 to 37,000 mg/l (El-Fadel and others, 1997:247) Critical review based on numerous studies.	Model value from mass basis while literature value in concentration (mg/L).

Methanogen u_{max} (d^{-1})	0.525	0.08 to 1.33 (El-Fadel and others, 1997:248) Critical review based on numerous studies.	Rates vary depending on composition of substrate and experiment. Lower value used to emphasize field conditions vice optimal laboratory conditions.
Methanogen Y	0.4	0.4 to 0.6 (Gaudy and Gaudy, 1980:239-240)	Y value reflects lowest efficiency of converting substrate to energy.
Methanogen K (mg)	1000	2 to 3900 mg/l (El-Fadel and others, 1997:248) Critical review based on numerous studies.	Model value from mass basis while literature value in concentration (mg/L).
Aerobe to Acetogen Decay Rates (d^{-1})	0.1	0.1 to 6.1 (El-Fadel and others, 1997:247) Critical review based on numerous studies.	Based on fermentative bacterial rate. Only methanogen decay rates differed significantly to warrant a separate numerical value.
Methanogen Decay Rate (d^{-1})	0.01	0.01 to 0.04 (El-Fadel and others, 1997:248) Critical review based on numerous studies.	Only methanogen decay rates differed significantly to warrant a separate numerical value.
Initial Organic Waste Mass	1×10^{46}	---	Large amount required to preclude waste depletion in an unreasonably short period of time. See Structure Verification section.
Other Substrate Initial Masses	0	---	Although some amount of each substrate will be present, the initial masses were zero to ensure model simulated natural progression of degradation.
Stoichiometric Ratios	various	See Stoichiometric Section of Chapter 2.	
Moisture Content	40%	Can vary landfill to landfill.	See Environmental Parameter section of Chapter 2.
Temperature	20-60	See Environmental Parameter Section of Chapter 2.	Represents rise of temperature from ambient as microbial activity increases until rise in temperature can become inhibitory.

Optimal pH for methanogens	6.4-7.4	See Environmental Parameter Section of Chapter 2.	Outside optimal range, pH becomes inhibitory to methanogens.
u_{max} = maximum specific growth rate Y = yield coefficient (mass of bacteria per mass of substrate consumed) K = half saturation constant			

Several comments can be made regarding the parameter values chosen for the model when assessing their plausibility and subsequent verification. First, the constants used for a majority of these parameters are applied unilaterally for a general bacterial group such as acetogens even though the constants are often highly dependent upon species or substrate. In reality, the values for these constants vary according to the growth conditions present, the substrate consumed, and the particular bacterial species present in a landfill. Constants will be different for the countless species which make up a general bacterial category, such as acetogens, as well as each possible substrate consumed.

Furthermore, the parameter values that have been found in literature will also vary according to the conditions of the experiment or field test present in assessing the values. For example, half saturation constants will vary according to the substrate consumed and the bacterial species, yet the model only applies a single half saturation constant for a bacterial group made up of countless species. The constant is the same regardless of the substrate. Such simplifying assumptions are necessary due to the inherent monumental task in assessing each possible species of bacteria and corresponding uncertainty with respect to the consumed substrate which could exist within a landfill.

Secondly, the prevalent step down of the bacterial maximum specific growth rates, yield coefficients, and half saturation constants reflect the differences in efficiencies regarding bacterial groups. Generally, aerobic bacteria maintain the highest efficiency in degrading and utilizing organic material while methanogens are the least efficient. As the process moves from aerobic to anaerobic and finally to methanogenic stages, the bacteria for each step usually become less efficient and their characteristics normally reflect this phenomenon.

However, note that the hydrolytic bacteria maintain a maximum growth rate below that of the other anaerobic bacteria even though they are associated with a higher level degradative step. Unlike the other anaerobic bacteria of the model, hydrolytic bacteria do not gradually achieve their maximum growth rate. Instead, the bacteria reach it instantaneously since there is no lag time in reaching the maximum growth rate because of the enormous amount of substrate already available. The growth rate value for hydrolytic bacteria is artificially set at a lower value to offset the absence of a substrate availability mechanism as discussed in the Structure Verification section. Although the aerobic bacteria growth rate experiences similar effects regarding the lack of lag time in reaching maximum growth rate, its rate is not artificially lowered. The growth of aerobic bacteria is also governed by a more limiting substrate, oxygen, thereby negating the requirement for a lower artificial growth rate to offset any absence of a substrate availability mechanism.

Another failure in parameter verification can also be linked to the structural verification difficulty associated with substrate availability. As noted previously, an

extremely large amount of initial organic material was required to prevent waste depletion before reasonably expected. If a smaller amount is used to reflect the more realistic ratio of bacterial mass to organic mass of 8 to ten orders of magnitude (depending on soil/waste type and cell attributes such as cell density), organic waste is depleted much faster than normally expected given the initial conditions of the model (Atlas and Bartha, 1993:193-194). Figures 21 and 22 illustrate the difference of how quickly organic solids (organic waste + simpler substances from the model) are depleted depending on the initial amount of organic material present.

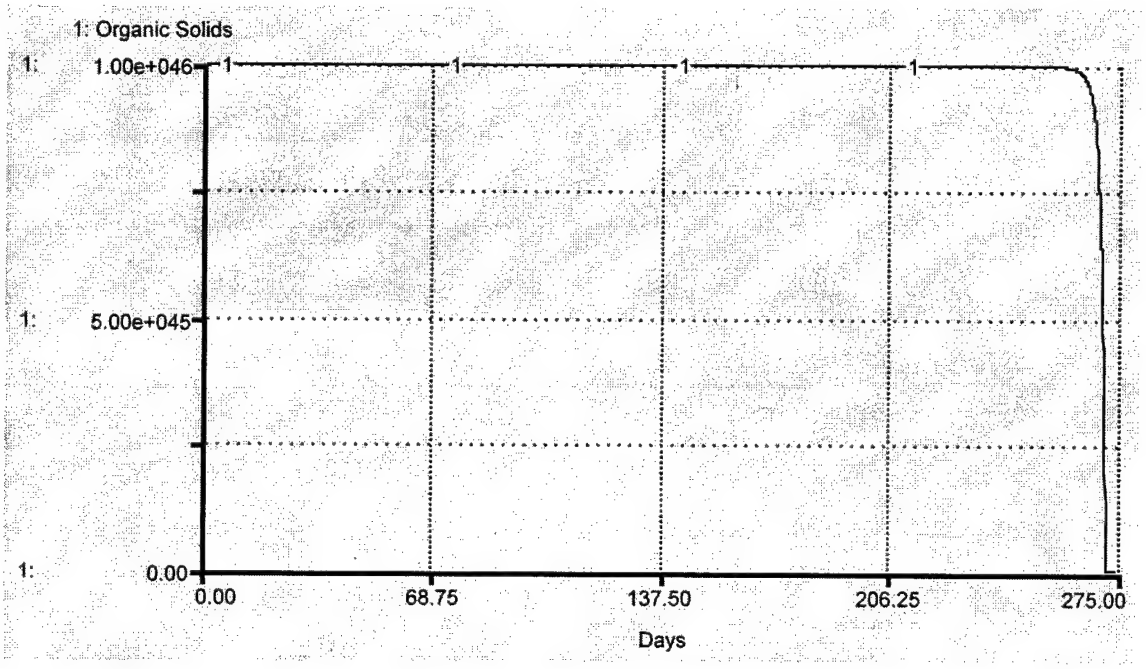


Figure 21. Organic Solid Depletion: High Initial Amount of Solids

Figure 21 shows how large the initial amount of organic material must be to prevent rapid depletion of the organic material in an unreasonably short period of time. Figure 22 demonstrates how quickly the organic waste is depleted given a ratio of organic

material to initial bacterial mass commensurate with a more realistic representation of such a ratio for an actual landfill. However, organic materials are not normally consumed or converted in the short period of time associated with Figure 22 given the initial conditions of the microbial environment for this model.

Again, the source of such a discrepancy in the plausibility and reasonableness of the initial value for organic material used in the model can be traced back to substrate availability. A properly designed mechanism addressing substrate availability inserted into the structure could correct the disconnect between amounts of organic material/substrate and depletion times for a reasonable initial mass of organic material and subsequent ratio of organic material to mass of bacteria.

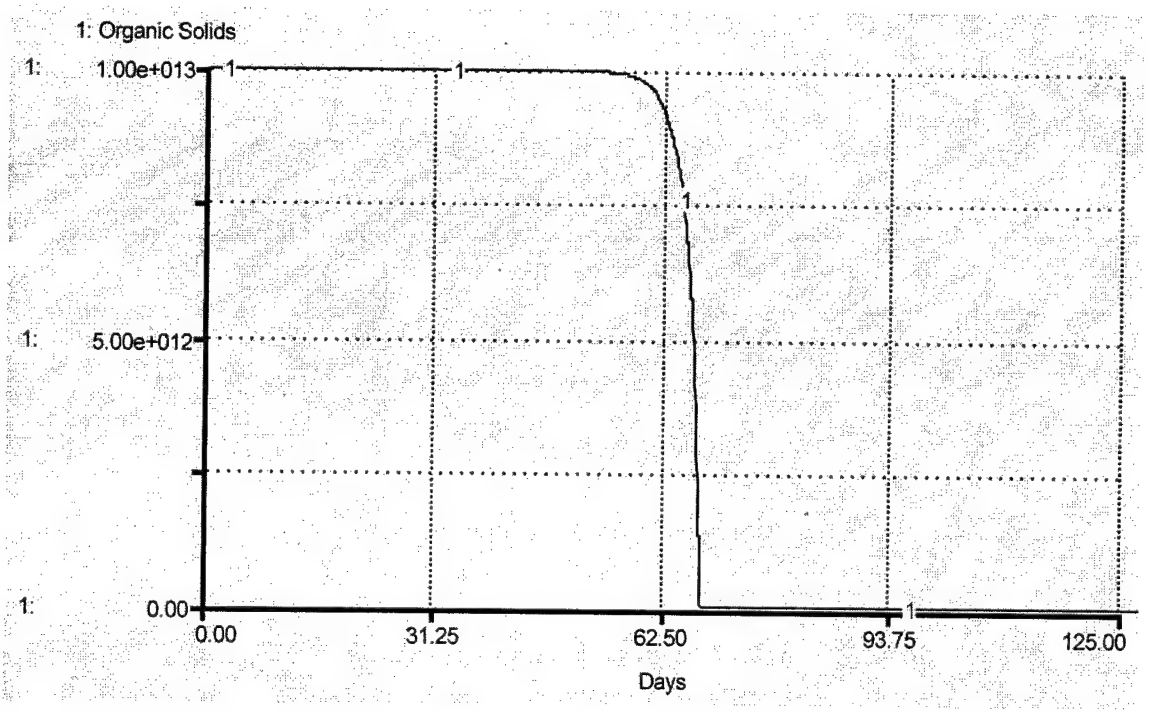


Figure 22. Organic Solid Depletion: Low Initial Amount of Solids

Lastly, the model employs parameter values based on mass units in accordance with its mass basis structure. For the stoichiometric ratios, the mass basis proves ideal in simplifying the determination of these ratios through equation balancing and molecular mass comparisons. However, the Monod biokinetic constants such as the half saturation constant are normally presented in concentration terms, making it more difficult to verify parameters numerically from the model's mass basis point of view. Although some constants such as maximum specific growth rates do not depend on concentration formulation, the parameters involved with Monod kinetics are generally derived in terms of concentration. The difficulty in assessing the accuracy of constants normally found in concentration terms but employed in mass terms for the model becomes another focal point for the future study and improvement of this model.

Extreme Conditions. For extreme conditions testing, model rate equations are examined to see which variables the equation depends upon, and these variables are tested at minimum and maximum values. The rate equations of this model (substrate depletion and bacterial growth) can ultimately be traced back to the levels and parameters defining bacterial growth to include substrate and bacteria stocks and the variables associated with the environmental parameters of moisture content, temperature, and pH. Not only do these entities define the crucial rate equations of the model, but many of these entities actually have the potential to exist at extremes depending on a particular landfill's conditions. Successful testing should result in expected plausible behavior for the model based on the extreme condition implemented. To simplify graphical

representation of the test results, when appropriate, only one type of bacteria and its related behavior are represented in a particular graph.

Substrate/Bacteria Stock Level. To test the stock levels driving bacterial growth, the stock levels determining the ratio of organic material to bacteria level were changed to represent extreme plausible conditions for the mass of bacteria relative to substrate initially present in the landfill. The graphs of this test and many of the following tests utilize different output and time scaling in order to facilitate the explanation of the results. Again, such scaling is a result of the large initial numbers associated with beginning stock values and the first order nature of the rate equations.

Figures 23 and 24 display the effects of changing the initial value of bacteria present in the landfill on the fate of the bacteria itself and/or gas generation, in this case methanogens and methane generation. Trace 1 of both graphs illustrates model results when the initial stock level of bacteria is extremely low compared to the initial organic material present (ratio of organic material to bacteria is extremely high). Trace 2 represents results with initial bacteria levels within one to two orders of magnitude of the organic waste amount (ratio of organic material to bacteria is extremely low).

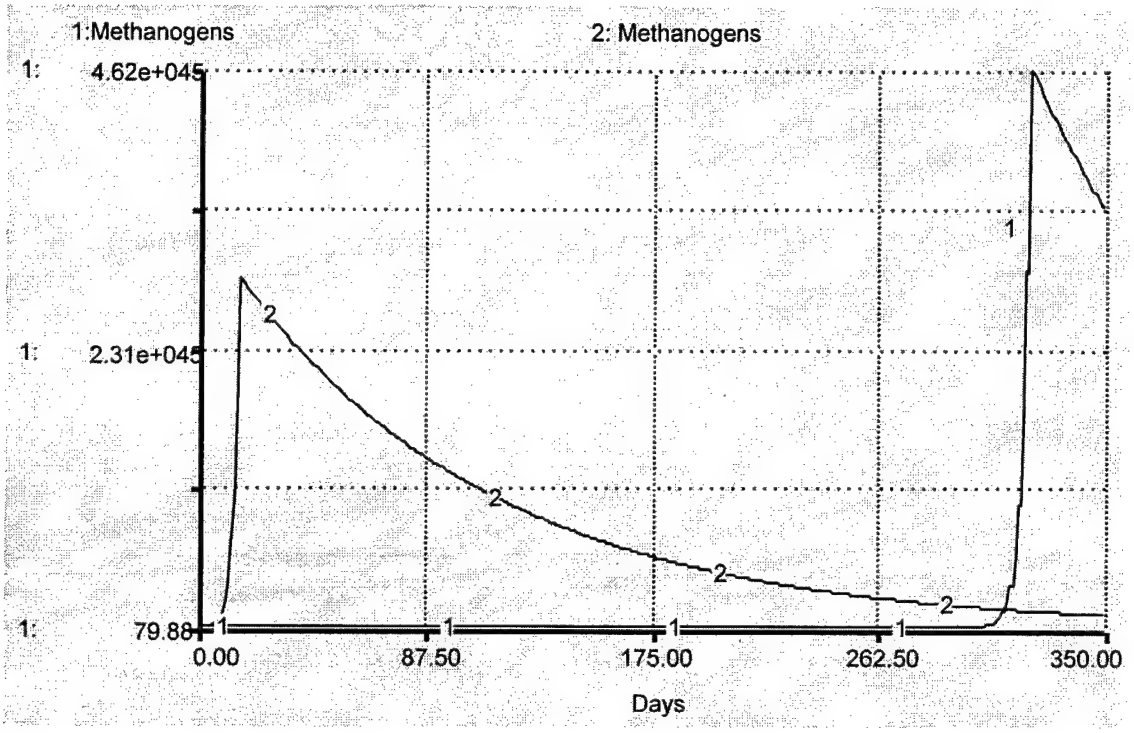


Figure 23. Extreme Conditions for Initial Stock Levels of Bacteria (Bacteria)

As expected, the bacteria population grows sooner if more bacteria are initially present since bacterial growth depends on the mass of bacteria present for growth. Moreover, the substrates required for methanogen growth are available sooner as the preceding substrates are converted much faster when larger initial masses of bacteria are simulated. However, the mass of bacteria differs by more than an order of magnitude when comparing peaks of bacterial mass. An initial lower bacteria mass prevents a rapid depletion of substrate since depletion is based on bacterial growth and ultimately accumulates a larger amount of bacterial mass *as long as the conditions and substrate quantity remain conducive to growth.* For both Traces, substrate becomes the limiting factor for overall bacterial mass. With larger initial amounts of bacteria, substrate is

depleted quicker, ending the growth of bacteria sooner. Figure 24 demonstrates the effect on gas generation.

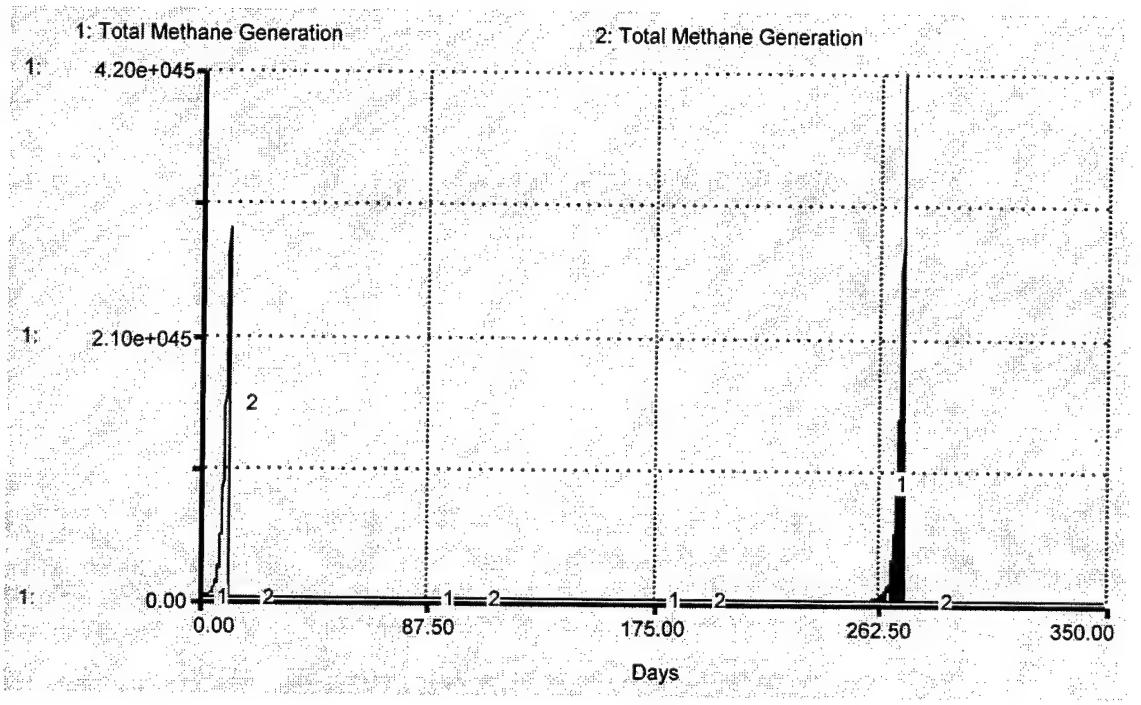


Figure 24. Extreme Conditions for Initial Stock Levels of Bacteria (Generation Rate)

Figure 24 demonstrates that gas generation also reflects the same phenomena seen in the bacteria mass graph of Figure 23. Although it seems logical for the total amount of methane generated to be higher with a larger amount of bacteria initially present (more organic material can be degraded sooner), more methane is actually generated in the long term with lesser initial amounts of methanogens present *as long as the conditions and substrate quantity remain conducive to growth,* albeit peaking much later. Again, degradation and subsequent gas generation become a question of substrate limitation; even if there is an enormous amount of bacteria present in the landfill, their ability to degrade material can be limited by substrate availability.

To summarize, this particular test confirms two key findings: if bacterial populations or mass can be increased to the highest levels by maintaining optimal growth conditions, substrate depletion and the gas generation associated with the depletion occur much faster. Secondly, substrate levels in the system (in both quantity and when they become available) can be critical in determining microbial growth thereby affirming the need to address substrate availability mechanisms in follow-on efforts in modeling degradation.

Moisture Content. Extreme initial moisture content levels of 0% (trace 1) and 100% (trace 3) were analyzed, and the base value of 40% (trace 2) is also graphed for use as a comparison tool). With no moisture, one would expect no bacterial growth or subsequent gas generation. Saturation conditions of 100% moisture should provide optimal growth conditions sooner and, thus, earlier gas generation. For this test, fermentative bacteria and carbon dioxide generation were utilized as examples. Figure 25 and 26 demonstrate carbon dioxide generation and fermentative bacteria.

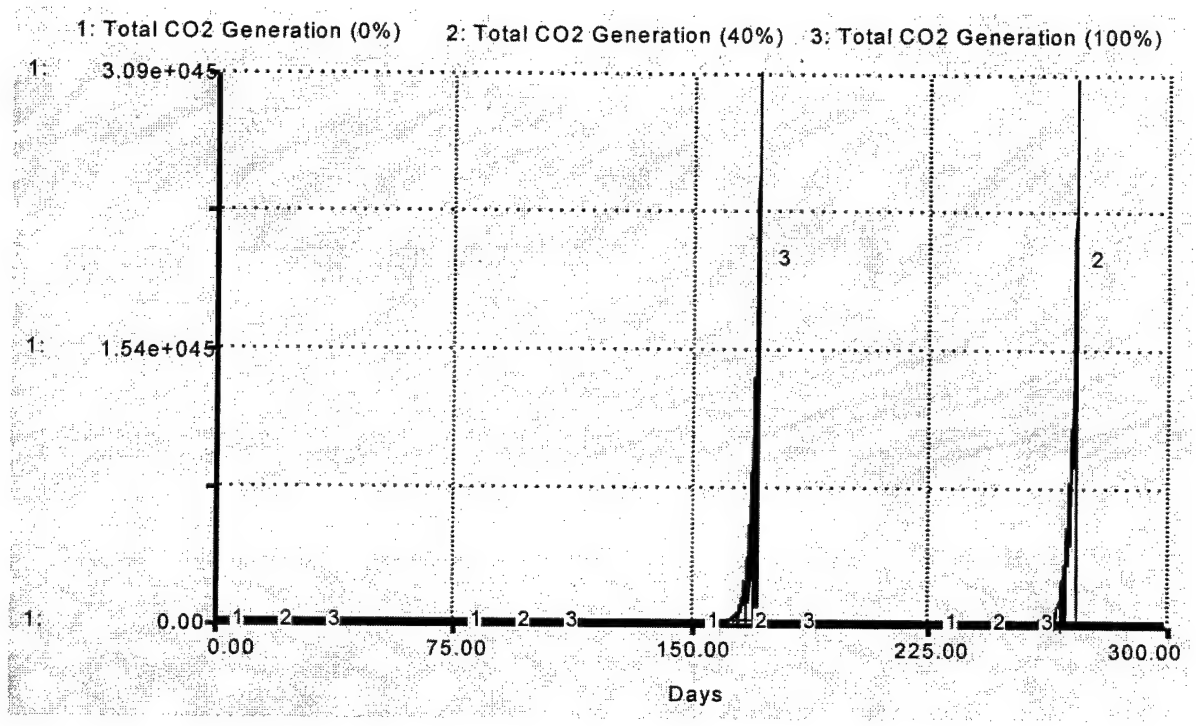


Figure 25. Carbon Dioxide Generation Under Extreme Moisture Conditions

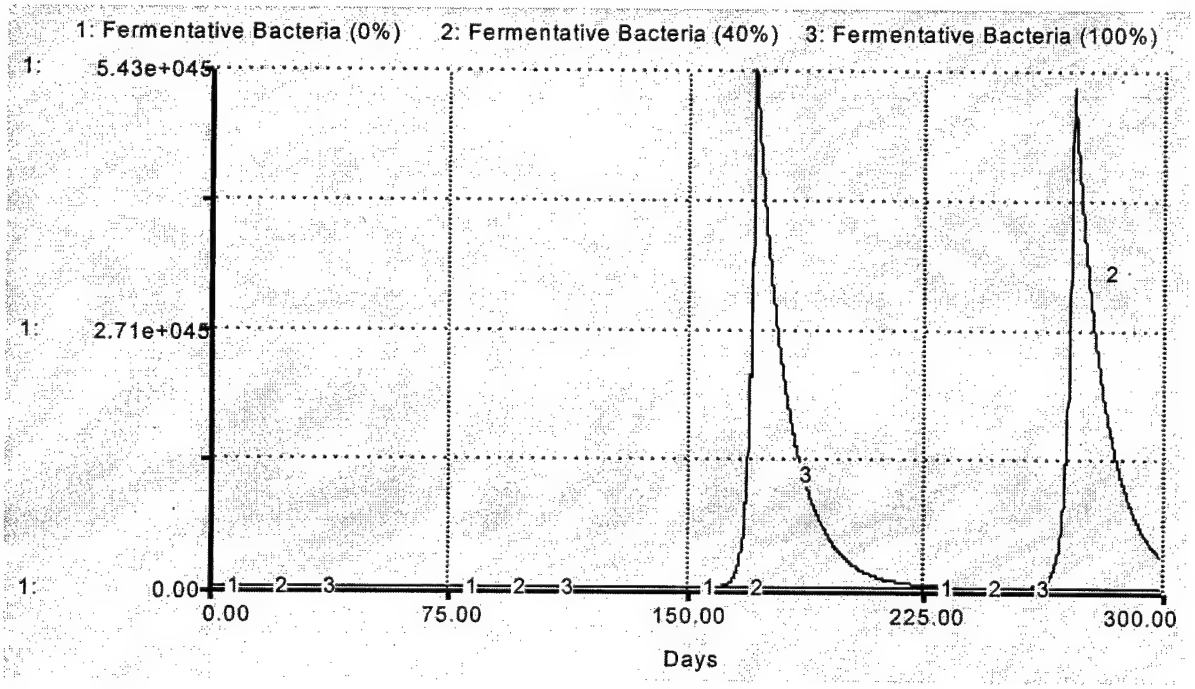


Figure 26. Fermentative Bacteria Under Extreme Moisture Conditions

As both Figure 25 and 26 illustrate, 0% moisture does result in no bacterial growth or gas generation. Saturated conditions (100% moisture) provides greater peak amounts of bacteria and gas generation sooner than a 40% moisture content. Saturated conditions accelerate growth and gas generation. This test affirms that extreme conditions of moisture provide plausible results for the model concerning the effects of moisture content on degradation.

Nutrients. The nutrient entity is modeled very simplistically with an "on/off" switch in the model, representing the presence or absence of required nutrients for bacteria survival and growth. The on/off approach is based on the observation that such nutrients are typically available from the waste within the landfill (Barlaz and others, 1990:575). There is no accumulation or depletion of these nutrients in the model; they either exist or are absent. In reality, some nutrients may be released from the substrate/microbe environment as either gaseous emissions or liquid-phase components of leachate, but such releases are accompanied by further breakdown of the complex waste matrix, making more nutrients available to the microbial population. For graphical presentation with Figure 27, acetogens are utilized for analysis, with trace 1 representing no nutrients and trace 2 available nutrients.

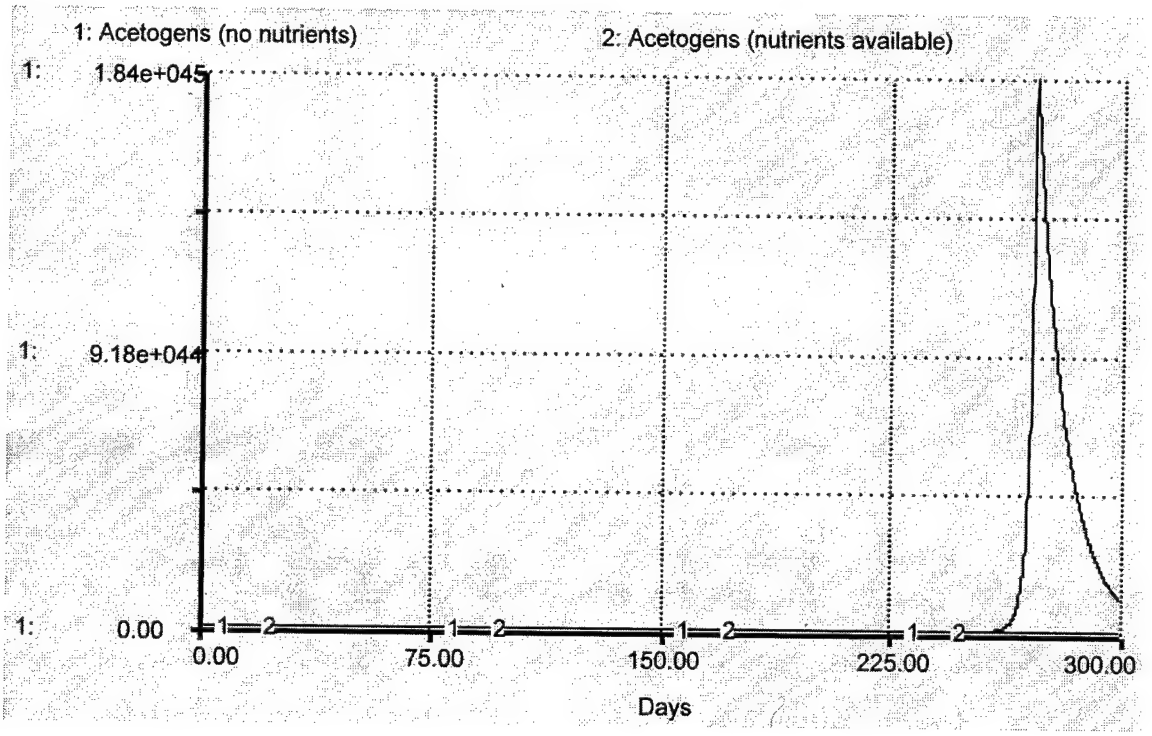


Figure 27. Extreme Nutrient Conditions

With such a simplistic approach to nutrient influence, it is no surprise that no nutrients results in no bacterial growth while available nutrients results in growth.

Temperature. To analyze the effects of temperature extremes, three different initial ambient temperatures were utilized: 0 deg C (trace 2), 20 deg C or baseline condition (trace 1), and 40 deg C (trace 3). Figure 28 demonstrates the results.

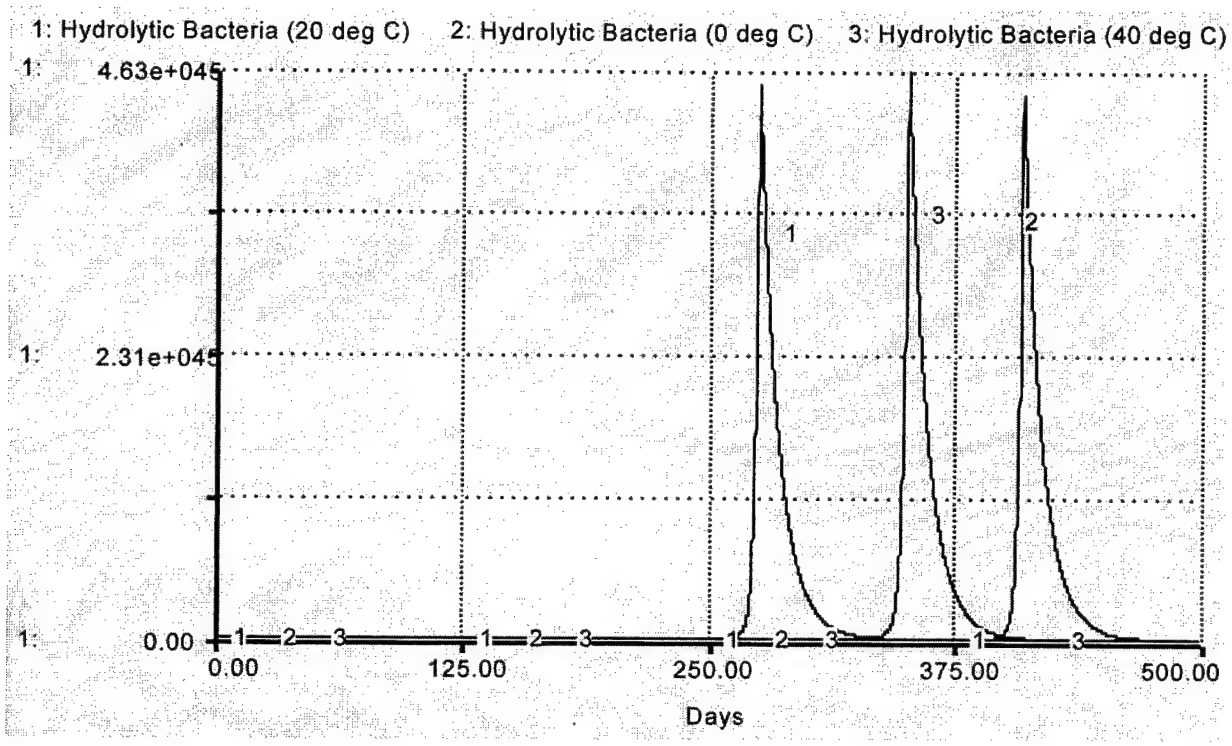


Figure 28. Effects of Extreme Temperature Conditions

It would seem logical that as the initial temperature is adjusted closer to optimum conditions for bacteria (assumed mesophilic and thermophilic conditions for the model), bacterial growth occurs sooner. The 0 deg C initial temperature does result in a lower peak of growth and more importantly, it takes longer for growth to peak. Microbial activity has to generate the heat necessary to raise the temperature. Such activity is inhibited at lower temperatures. However, an initial temperature of 40 deg C actually causes bacterial growth to peak later than 20 deg C. Although the 40 deg C temperature is initially optimal for the bacteria, it causes the bacteria to approach even higher temperatures faster, temperatures which begin to inhibit growth. Although the likelihood of experiencing 40 deg C temperatures as initial conditions for a landfill are remote, using

this extreme temperature points out a limiting factor for bacteria on both sides of the temperature spectrum. Yet, the question remains whether normal landfill conditions would ever allow such temperatures to be reached during degradation. The key is to improve upon the mechanism linking microbial activity to temperature beyond the simplistic graphical mechanism presently incorporated in the model.

Oxygen. Oxygen obviously inhibits the growth and ability to function of purely anaerobic bacteria. To subject the model to oxygen extremes, the oxygen entity was adjusted to simulate no oxygen present whatsoever in the waste (trace 1) and an extended amount of oxygen remaining beyond normal time limits (trace 3). Trace 2 is the baseline oxygen level used in the model. Figure 29 illustrates the result on the hydrolytic anaerobes.

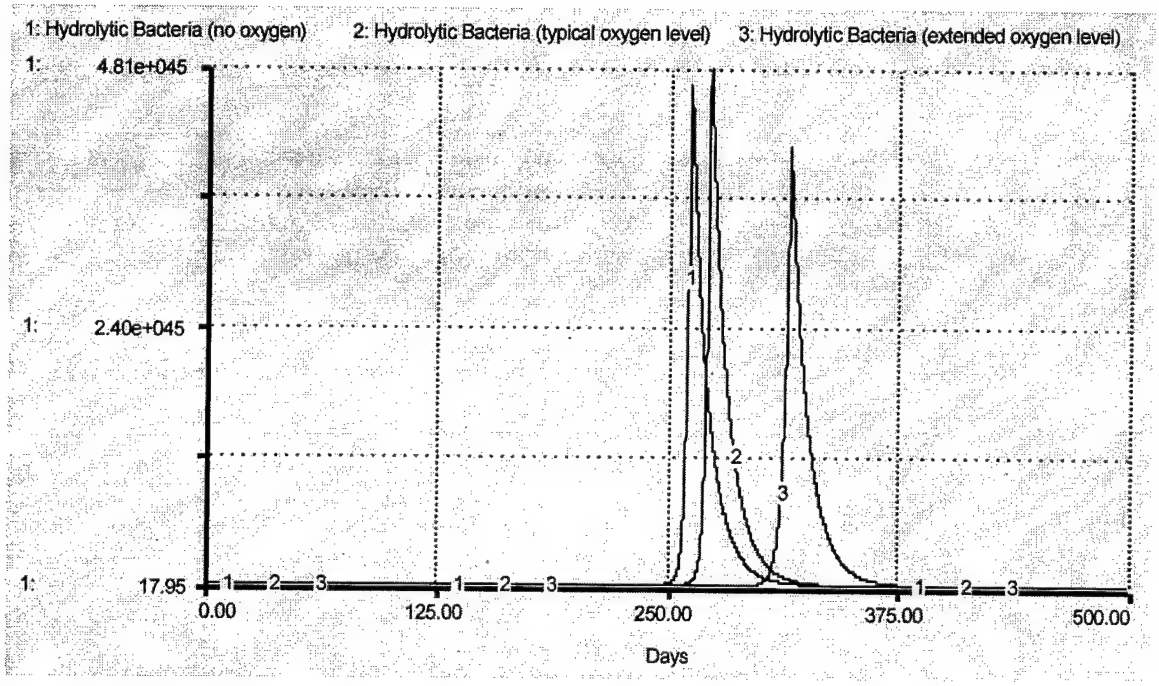


Figure 29. Effects of Extreme Oxygen Levels

With no oxygen present anaerobic bacteria begin growing immediately resulting in a peak of bacteria occurring earlier (as long as other conditions are favorable and substrate is available) than a system with typical or extended levels of oxygen initially present. If oxygen persists in the system, anaerobic bacteria will not grow until the oxygen is depleted as depicted by the delay in the peak of hydrolytic bacteria represented with trace 3. The bacteria eventually exceeds its decay once oxygen is depleted and undergoes rapid growth.

pH. The final extreme condition involves the pH of the organic material within the system. Since methanogens have been documented being the most sensitive bacteria to pH, pH is assumed to have its greatest effect on methanogens, and methanogens are used for analysis. Three conditions were simulated for this test: an initial basic pH beginning at 9.0 (trace 1); an acidic pH level of 6.0 simulating overproduction of acids by fermentative bacteria (trace 2) and; a completely inhibitory acidic pH level of 5.0 simulating overproduction of acids by fermentative bacteria (trace 3). All of these conditions are inhibitory to varying degrees for methanogens and, consequently, for methanogenesis based on the ideal range of pH for methanogenesis as discussed in Chapter 2. Figure 30 displays the result over the overall time period.

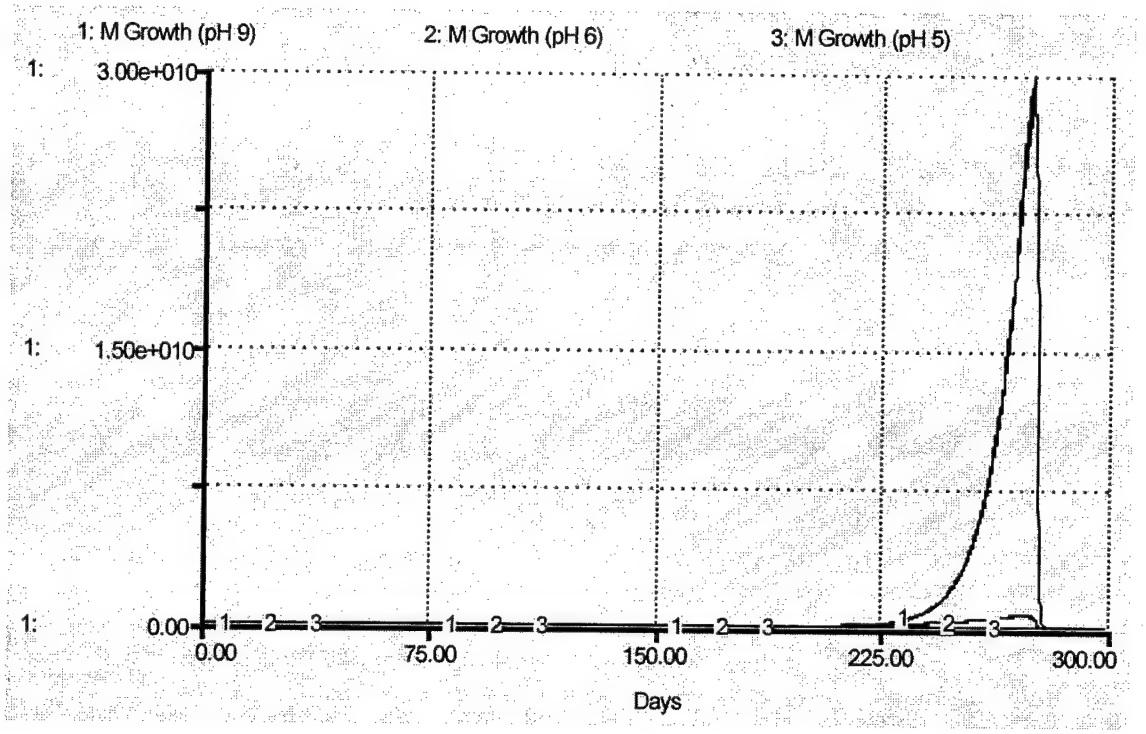


Figure 30. Effects of Extreme pH Conditions on Methanogen Growth

The basic condition initially inhibits growth, but acid production by fermentative bacteria, on which pH has little effect, eventually decreases the pH to levels more favorable for methanogen growth. Acidic conditions provide the opposite atmosphere. The acidic conditions detrimental to methanogens curtails methanogen growth, resulting in limited future growth as compared to growth under optimal conditions (a pH of 6.0 still offers very limited growth ability) or no growth as depicted by Figure 30, traces 2 and 3.

Another view of the same conditions can be simulated utilizing methanogens as the observed entity as in Figure 31.

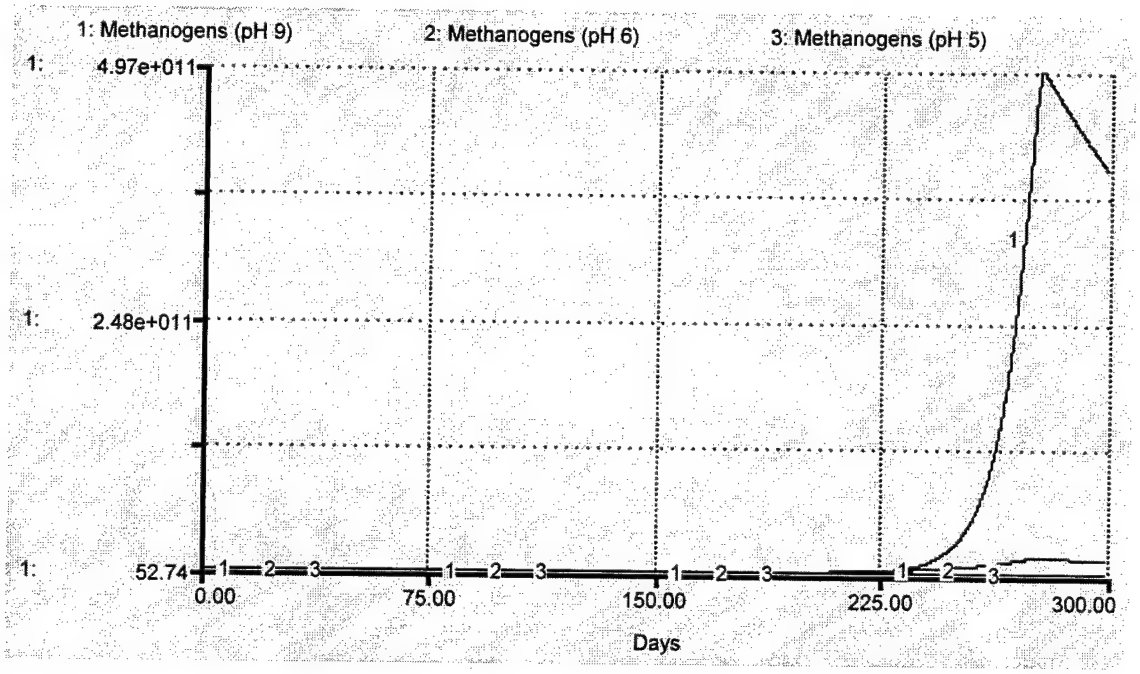


Figure 31. Effects of Extreme pH Conditions on Methanogens

Figure 31 confirms the reduced and zero amounts of methanogen mass due to inhibitory acidic conditions at pH levels of 6.0 and 5.0. With such results on methanogens, one would expect similar results from methane generation. Figure 32 demonstrates similar results for methane generation.

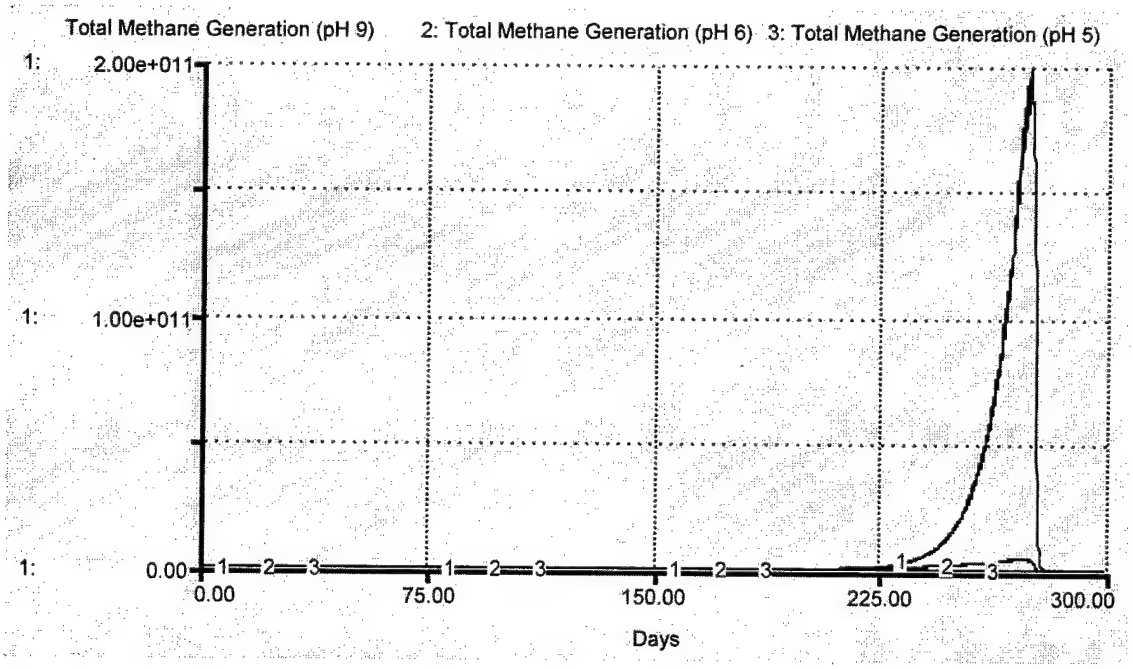


Figure 32. Effects of Extreme pH Conditions on Methane Generation

Although extreme pH condition testing, even with the simplistic graphical mechanisms employed by this model in relating acid production to pH levels, affirms the detrimental and limiting effects of certain pH levels on methanogens, it also demonstrates the effects of substrate depletion. Growth occurs, even if limited by acidic conditions just outside the optimal pH range for methanogens such as a pH of 6.0 as long as substrate and other environmental conditions allow for it to continue. (Certain pH levels such as 5.0 will be detrimental to methanogens regardless of other conditions.) Lastly, consideration should be given to utilizing a concentration based model in future efforts to better represent mechanisms governing concentration related entities such as pH.

Boundary Adequacy. The boundary adequacy test determines whether the level of model aggregation is appropriate given the model's purpose. Is additional structure

required for the model to adequately fulfill its purpose? Such additions to the model should arise from a developed plausible hypothesis which proposes additional structure is needed in examining the issues addressed by the model. To illustrate the importance of such testing, consider the initial structure of an earlier version of the model for this thesis. The earlier version consisted of a structure dividing the biodegradation process into only two distinct phases, aerobic and anaerobic, combining all the anaerobic degradative steps of the current model structure into one major category and utilizing only organic waste as the substrate for all degradative steps.

Through simulation of the earlier version of the model and additional literature review, it is apparent that the level of aggregation associated with such an approach does not adequately incorporate the interrelationships and interdependencies between the various bacteria involved in degradation as organic waste is consumed and converted. Simulation confirmed the alteration in behavior when the anaerobic phase of the earlier version of the model was changed to reflect a more detailed view of degradation by inserting additional degradative steps. Figure 33 illustrates the change utilizing the entity of carbon dioxide and the addition of the hydrolysis step as the example.

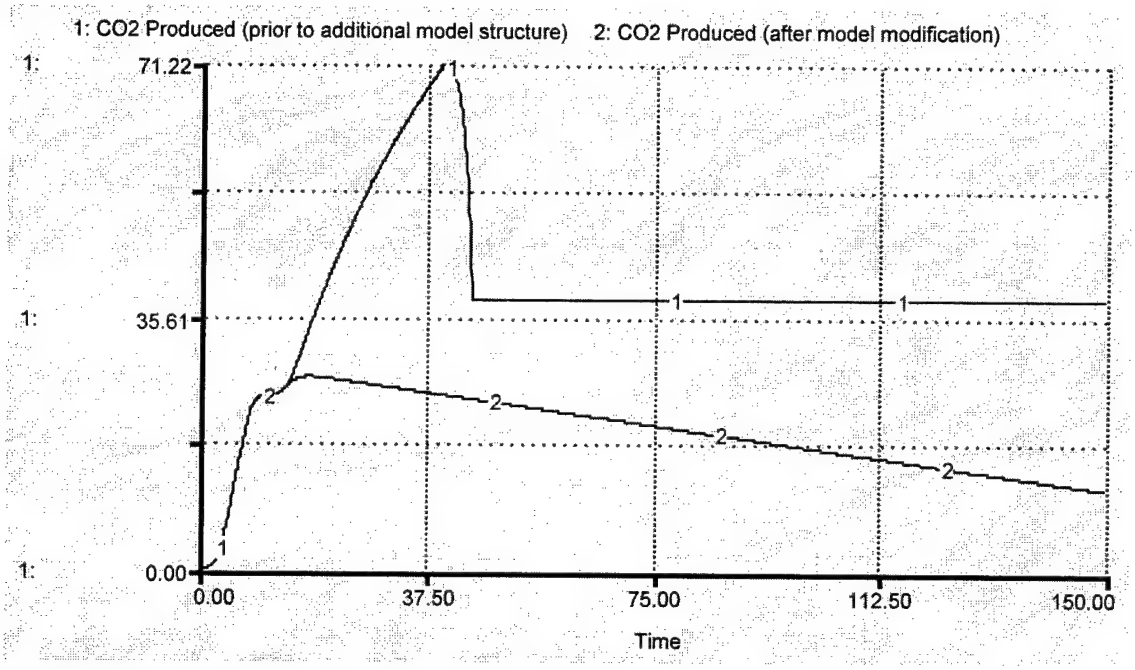


Figure 33. Change in System Behavior Due to Additional Model Structure

As Figure 33 shows, behavior for the mass of carbon dioxide was significantly altered as its dependence shifted to another substrate (simpler substances) instead of depending solely on organic waste. Further literature review and repeated simulations involving additional degradative steps resulted in the current level of aggregation used in the model in focusing on the model's purpose of simulating the fundamental processes of degradation. However, the current model's level of aggregation can also be tested for adequacy by addressing other plausible hypotheses regarding the inclusion of other entities thought to have significant influence on system behavior.

One such hypothesis involves the presence of sulfate within the landfill waste. It is well understood that sulfates in the waste stream can result in the generation of H_2S gas, an obnoxious gas constituting a small part of total of landfill gas produced. Not only

does this hypothesis include sulfate, but it can be expanded to include other electron acceptors available in the landfill. The presence of sulfate may generate significantly different degradation behavior from the model and require the addition of such structure to the model. Sulfate reducing bacteria can outcompete methanogens for substrates, thereby restricting methanogenesis (Gurijala and Suflita, 1993: 1178-1180). Sulfate does not directly affect the methanogens, but inhibits their growth by providing a more energy favorable pathway for electron flow (Widdel, 1988:507). Therefore sulfate reduction will occur prior to and at the expense of methanogenesis.

To test the influence of sulfate bacteria on overall system behavior, the following stoichiometric equations were incorporated into the model along with the appropriate sulfate reducing bacteria structure (Widdel, 1988: 494).

$$CH_3COO^- + SO_4^{2-} \xrightarrow{\text{Sulfate Reducing Bacteria}} 2HCO_3^- + HS^-$$

$$4H_2 + SO_4^{2-} + H^+ \xrightarrow{\text{Sulfate Reducing Bacteria}} 4H_2O + HS^-$$

Parameter values for the sulfate reducing bacteria reflect the tendency of sulfate bacteria to maintain higher biokinetic constants than methanogens. Figure 34 displays the behavioral results of adding the sulfate structure to the model. Trace 1 represents methane generation without sulfate present initially, and trace 2 is with the sulfate structure.

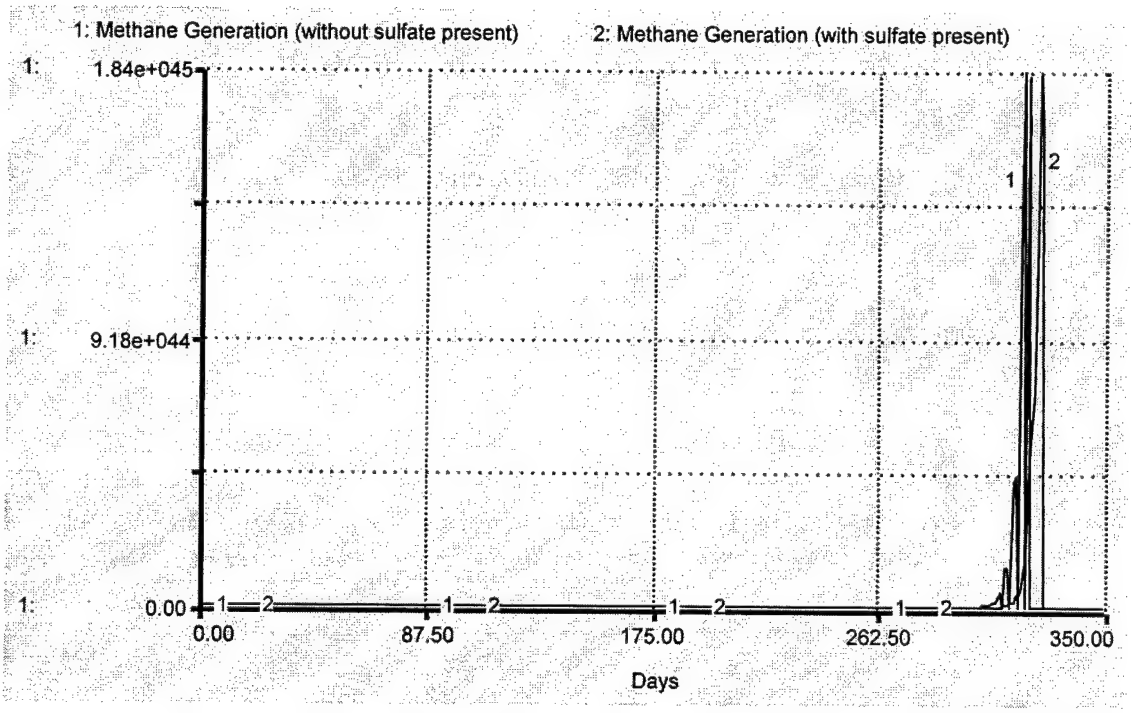


Figure 34. Effects of Adding Sulfate Structure to Model

Figure 34 illustrates the results of adding the sulfate structure. As expected, the sulfate slows the rate of methane generation, but only slightly, and has little effect on the peak of methane generation. Most importantly, the general behavior of methane generation for the system did not change significantly. The existence of several alternate electron acceptors within the landfill and their combined effects (depending on their availability) could slow generation rates even further. However, most alternate electron acceptors such as sulfate or nitrate are depleted quickly and normally exist in relatively small quantities.

Behavior Reproduction and Prediction Testing. Behavior testing addresses how well model generated behavior matches the behavior of the real system. Such testing can be divided into two major groups, behavior reproduction and behavior prediction,

depending on whether one is interested in historical or future behavior of a system. For the degradation system, both types of testing are applicable. Of the numerous behavior reproduction tests available, the relative phasing test proves most applicable in testing a real system which involves processes occurring in phases. Similarly, the pattern prediction test also proves most applicable since it attempts to examine whether a model generates the qualitative patterns of future behavior by evaluating phase relationships.

The model output can be analyzed from both the reproduction and prediction viewpoints. Although the model is not specifically tied to a unique historical system, the current representations of degradation and, consequently, gas generation are based on collected historical, empirical data. Moreover, even though the representations are derived from historical data, such representations offer predictive qualities in presenting future patterns of behavior since the overall basic processes and progression of degradation remain essentially unchanged regardless of whether the past or future is being examined. Both the relative phasing and pattern prediction tests provide a similar focus in testing behavioral confidence concerning phase relationships for the model. Thus, behavioral testing will address both areas of testing with one set of model output, concentrating on the phase relationship aspect of both tests.

Phase Relationship Testing. By observing the model output of how degradation progresses, one can determine whether the model captures the degradative steps observed in real decomposition systems. For both Figures 35 and 36, a smaller amount of initial organic waste is utilized for the simulation to ensure the plots can maintain the scaling required to include all of the appropriate entities for this particular

behavioral test. Figure 35 illustrates the model output delineating the overall progression of degradation as represented by the substrates of the system.

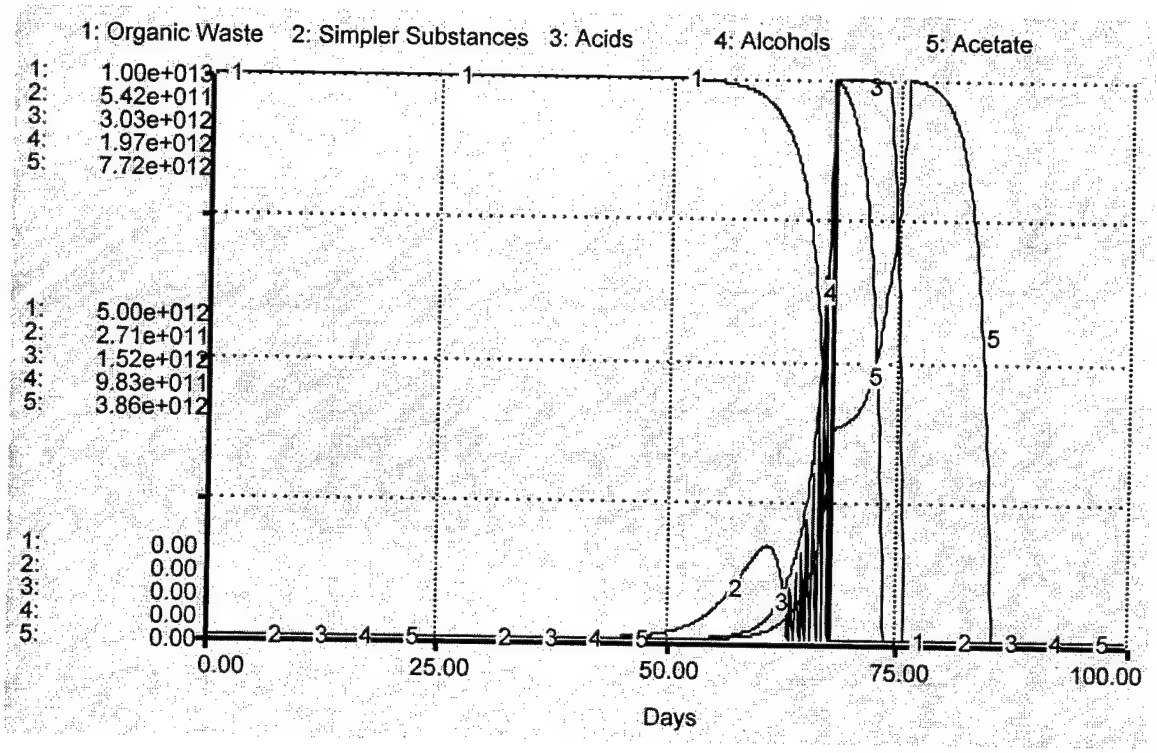


Figure 35. Progression of Degradation

Figure 35 illustrates the natural progression of degradation alluded to in the literature. Moreover, this graph displays how acetate is produced by fermentation as well as acetogenesis. Although the stock for simpler substance fluctuates due to the fluctuations in bacterial growth (addressed in Behavior Anomaly section), the general trend illustrates the substrates are depleted in the order they would be consumed or converted in the decomposition process. Figure 36 also demonstrates the relative phasing of the degradation process by depicting the bacterial groups responsible for converting the

substrates of the bioreactor system. The bacteria peak in succession following the availability of their particular substrate.

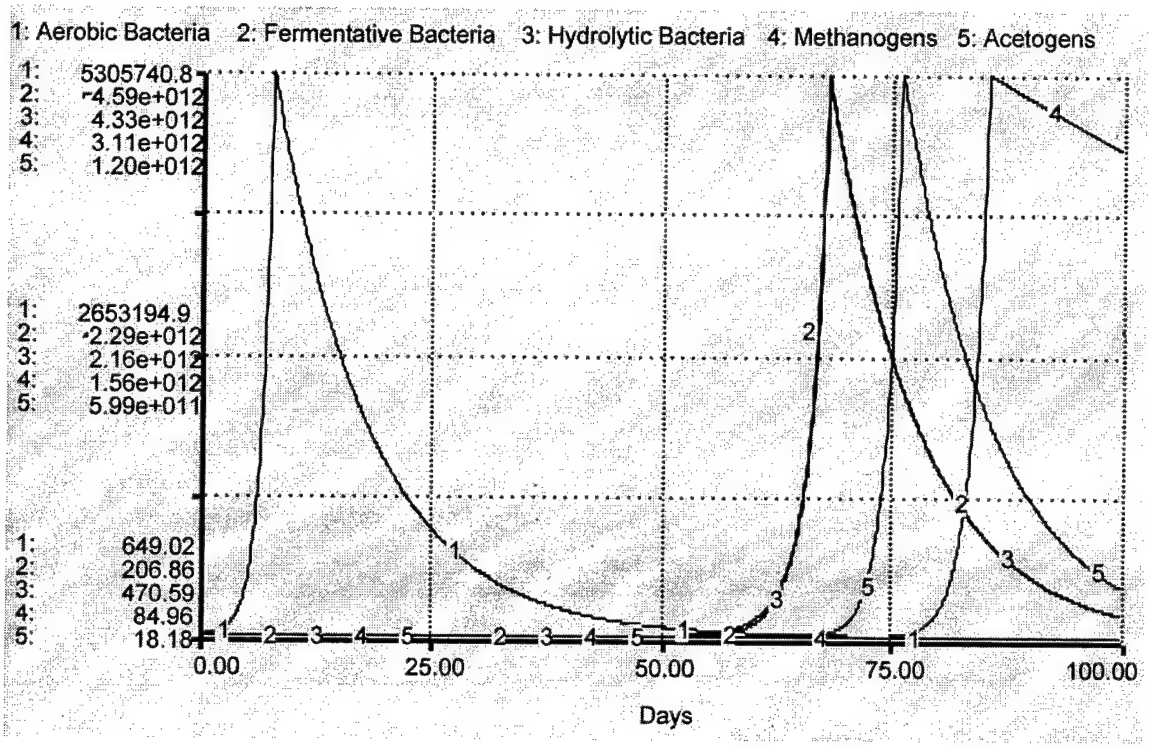


Figure 36. Bacteria Responsible for Degradation

Another way to view relative phasing is to examine the growth rates concerning the various bacteria involved as depicted in Figure 19. In general, the growth rates are consistent with the natural progression of the system except hydrolytic and aerobic bacteria as discussed in the Structural Verification section of this chapter.

As degradation proceeds from phase to phase, new substrates are available in greater amounts, so the bacteria responsible for continuing the process overtake the earlier dominant species and eventually achieve their maximum growth rate. Figures 19 and 36 demonstrate this behavior.

Another way to examine the behavioral progression is to view output of the model concerning the relationship between bacteria and the substrate consumed. The bacteria should continue to grow until their respective substrate is depleted. Viewing model output which addresses the relationship between bacteria and substrate also emphasizes the dependency of each set of bacteria on the previous bacterial group to function properly. Otherwise, if one step of the process is not carried out, the subsequent substrate will not accumulate, limiting the proper functioning of the bacteria dependent on the substrate. Thus, the degradation process will not be carried out to completion. Figures 37 through 41 depict each bacteria group and its relationship to a substrate.

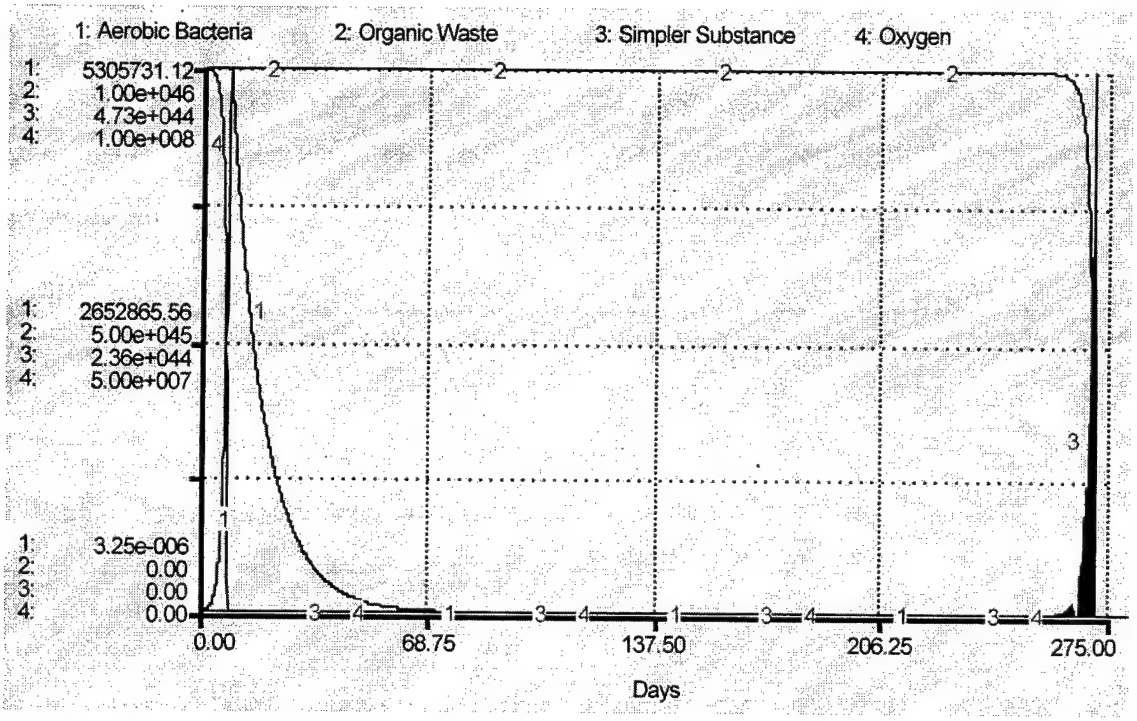


Figure 37. Relationship Between Aerobes and Substrates

The aerobic bacteria do not decline in concert with the organic substrates they utilize for energy, but instead begin their decline after the oxygen is depleted. This behavior is confirmed in actual degradation, as most soluble material which can be consumed by aerobes remains long after oxygen depletion leads to aerobe depletion.

Hydrolytic bacteria depend on complex organic waste for energy, thus the stock of hydrolytic bacteria increases until all of the organic waste is degraded. (See Figure 38.) The simpler substances they produce become the energy source for fermentative bacteria.

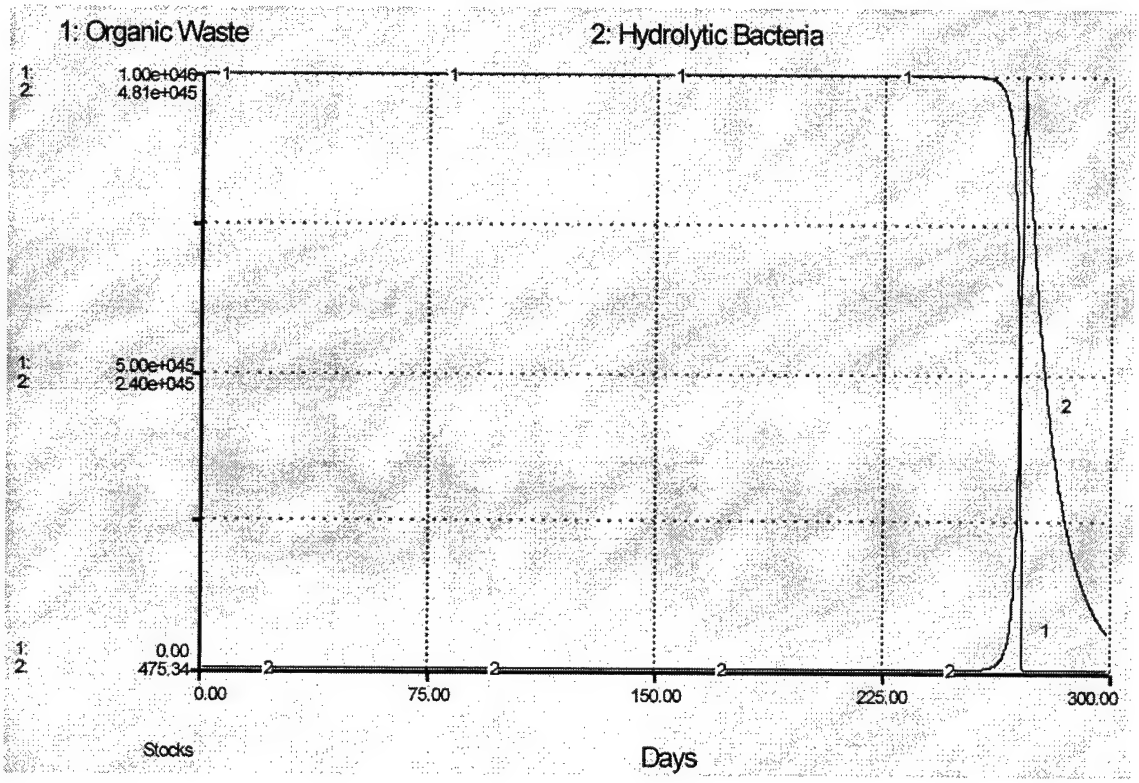


Figure 38. Relationship Between Hydrolytic Bacteria and Substrate

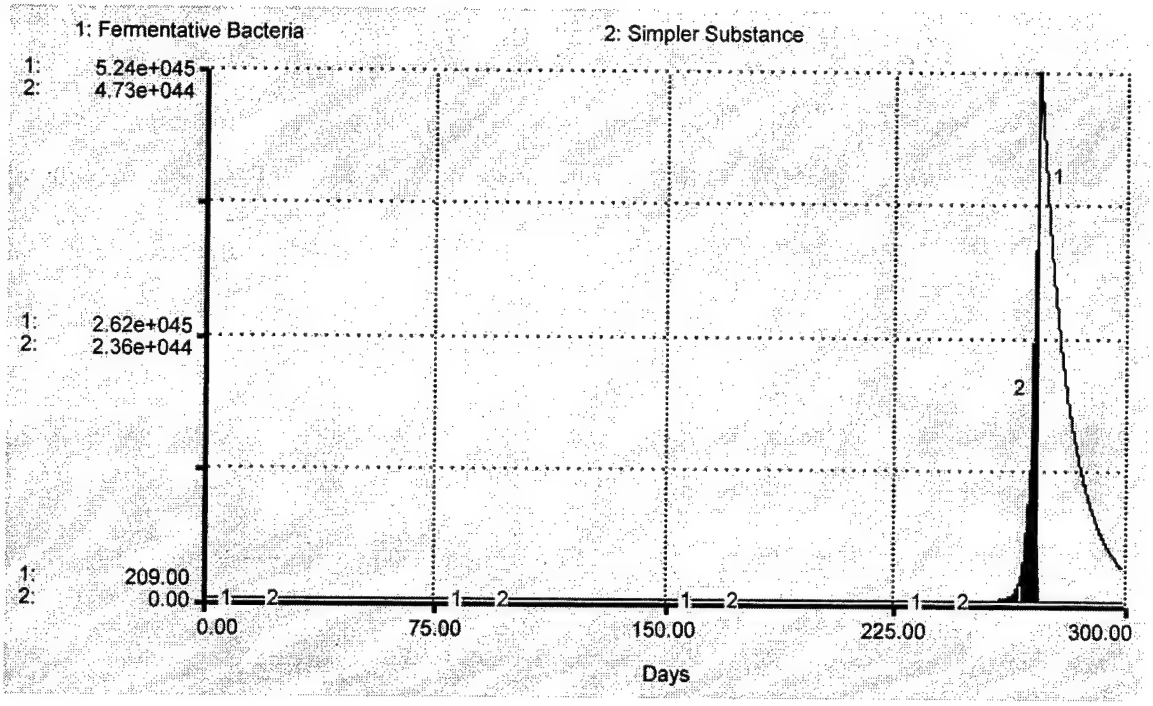


Figure 39. Relationship Between Fermentative Bacteria and Substrate

As depicted in Figure 39, the fermentative bacteria also grow until their particular substrate is depleted. Although the simpler substances fluctuate, the stock maintains an overall increase until it is completely depleted by the enormous amount of fermentative bacteria mass that has accumulated. After fermentation, several substrates (acids, alcohols, acetate, etc.) are available for the subsequent bacterial groups.

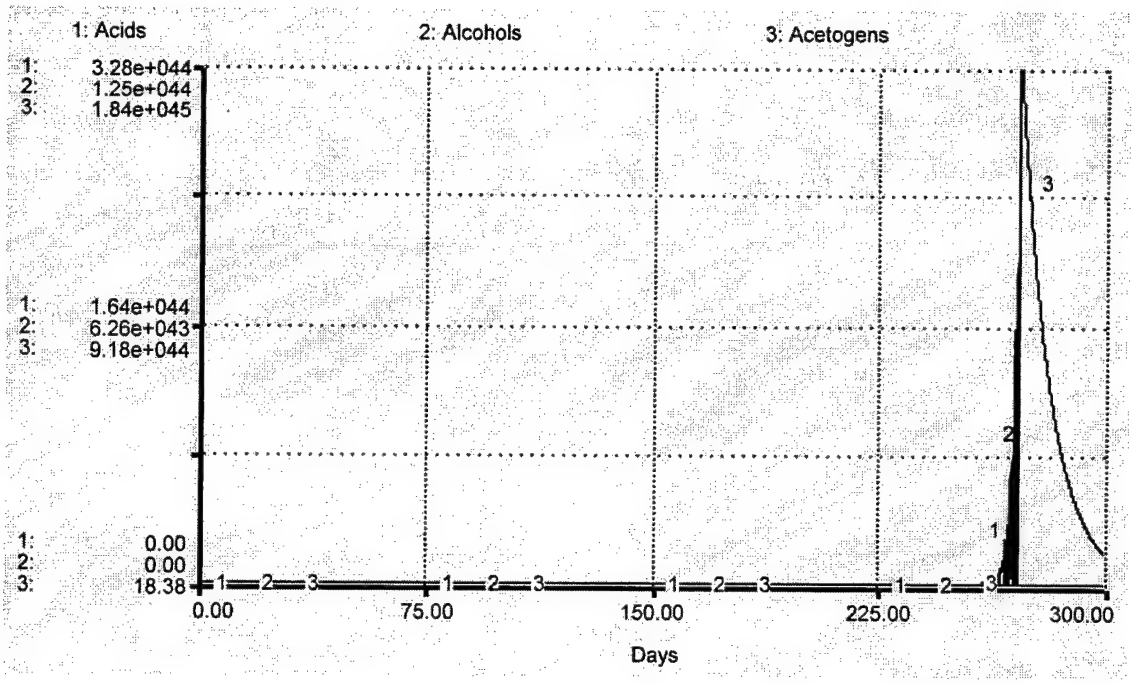


Figure 40. Relationship Between Acetogens and Substrate

For acetogens, both alcohols and acids are available for consumption. Since either substrate can sustain the bacteria, the acetogens do not decline until both substrates have been depleted and converted to other products.

Lastly, methanogens rely primarily on acetate for energy but can also utilize the substrate combination of $H_2 + CO_2$ for energy. Since acetate is the primary substrate for methanogens, Figure 41 illustrates the decline of methanogens once the acetate is depleted.

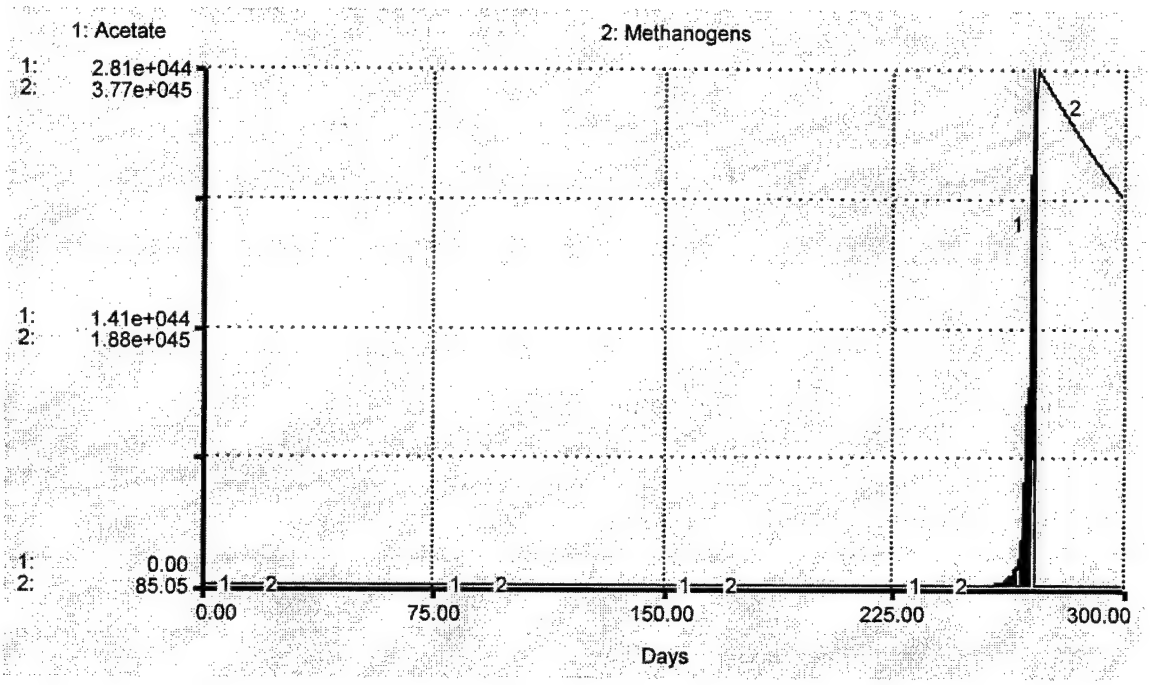


Figure 41. Relationship Between Methanogens and Substrate

Figures 37 through 41 are presented to depict how model generated behavior compares to the observed behavior of real systems. The graphs illustrate the criticality of the interrelationships that exist between the various bacteria and their functions in the chain of decomposition. Certainly, the general behavior of progression associated with the phase behavior of actual degradation has been portrayed by the model generated output. However, the shape of the behavioral curves of the model output entities may not be an exact match of the behavior found in decomposition processes. Much of the observed behavior of actual degradation systems depends on transient landfill conditions and initial waste composition, but, the general trends of degradation and phase relationships between variables have been captured. More importantly, the behavior arises as a consequence of model structure without the aid of an exogenous time series

input such as a periodic addition of moisture from an external source to drive model behavior. The model relies on the interdependencies associated with the system, interdependencies crucial to the real system as well.

Behavior Anomaly Testing. Anomalous behavior testing attempts to address any aberrations in behavior of the model output. Although one expects any model to operate (and thus produce behavior) similar to the real system, often times, a model generates unforeseen behavior. Furthermore, anomaly testing can be used to justify the use of certain assumptions if changing those assumptions results in anomalous behavior.

Anomalous Behavior Discovery. As alluded to in previous sections regarding testing, anomalous behavior was discovered with respect to certain instances of substrate depletion and gas generation. The behavior demonstrated fluctuating tendencies, although the anomalous behavior inevitably followed the overall general trend of behavior associated with the entities under consideration. Unfortunately, due to software limitations (see Conclusion section of this chapter), the scaling required to view such fluctuating behavior in detail does not allow for the detailed plots to be imported into the document. Fluctuating behavior can only be denoted by model behavior which appears "filled in" in the plots already shown.

By tracing back through the various relationships involved, it was discovered the anomalous behavior originated with the certain bacterial growth behavior. If one focuses on the "filled-in" appearance of the substrates, Figures 39 through 41 somewhat demonstrate the fluctuating growth of the bacteria represented in the model. When viewing detailed graphs of these same plots (plots not shown), the fluctuating bacterial

growth and substrate stock levels becomes more pronounced. Aerobes and hydrolytic bacteria are not addressed as their growth did not generate such anomalous behavior. The behavior appears anomalous because of the nature of the bacterial growth: falling to zero and then increasing to a larger amount almost instantaneously. Such fluctuations in growth affect substrate depletion, which eventually affects the following set of bacteria depending on the product of the reaction in progress. Thus, fermentative bacteria begins the anomalous behavior, and it continues through methanogenesis.

The root cause for such behavior seems to stem from the strong relationship between bacterial growth and substrate depletion dictated by Monod kinetics. As the bacteria undergo rapid growth, depletion also rapidly increases. So much, in fact, that at times the substrate is not allowed to accumulate before it is consumed by the bacteria. When the substrate is gone, bacterial growth immediately feels the effect. Thus, the alternating fluctuations between bacterial growth and substrate occur. The overall increasing trend results from the previous reaction continuously feeding the following degradative step. For example, hydrolytic bacteria continue to grow and break down organic material into simpler substances for the fermentative bacteria, thereby sustaining the overall growth of fermentative bacteria and accumulation of simpler substances.

Although the graphs still illustrate the interdependencies of bacteria on both their substrate and the preceding group of bacterial reactions, clearly such rapid rises and falls in growth and substrate levels do not appear to be indicative of the real system of biodegradation. It appears the anomalous behavior may be tied to the relationship between bacterial growth and substrate depletion. However, it must be emphasized that

since the modeling software utilizes numerical integration methods, the anomalous behavior may be caused by hardware limitations that do not allow for the appropriate integration step times for model simulation. When integration times are too large during model simulation, the fluctuating behavior referred to may result. In exploring the anomalous behavior, the hardware limitations should be examined first. Otherwise, the answer may lie with addressing substrate availability (if not all substrate is available for consumption, substrate levels and bacterial growth would not fluctuate as wildly), but the ramifications of addressing the substrate availability mechanism will not be known until the requisite improvement is incorporated into the current model.

Assumption Justification. Determining plausible values for the biokinetic constants employed by Monod kinetics can be difficult since most values cited in literature are derived from empirical data from laboratory or field experimentation under very specific conditions. The detection of anomalous behavior allows one to narrow down the range of plausible values by noting which values result in abnormal behavior for the system. Maximum specific growth rates play a significant role in determining the rate of substrate depletion and subsequent progression of degradation. Remembering that the initial amount of organic material employed by the model is uncharacteristically large compared to the initial mass of the bacteria of the system, the maximum specific growth rates were varied using the literature values as guidelines to aid in their value determination. Specifically, these values for maximum growth rates were judged for plausibility by whether or not the organic material was being consumed in a timely fashion given the other initial conditions and assumptions of the system.

In most biodegradation experiments investigating growth rates and utilizing Monod kinetics, the maximum specific growth rate is given in per-hour units and are typically on the order of 0.5 /hr. Converting those experimental values to the model's per-day dimensions yields maximum growth rates on the order of 12.0 /day. Employing this value for the bacterial growth rate results in the organic material of the system being depleted within a few weeks (see Figure 42), an unreasonable outcome given the large amount of initial organic material in the system and our understanding of landfill systems.

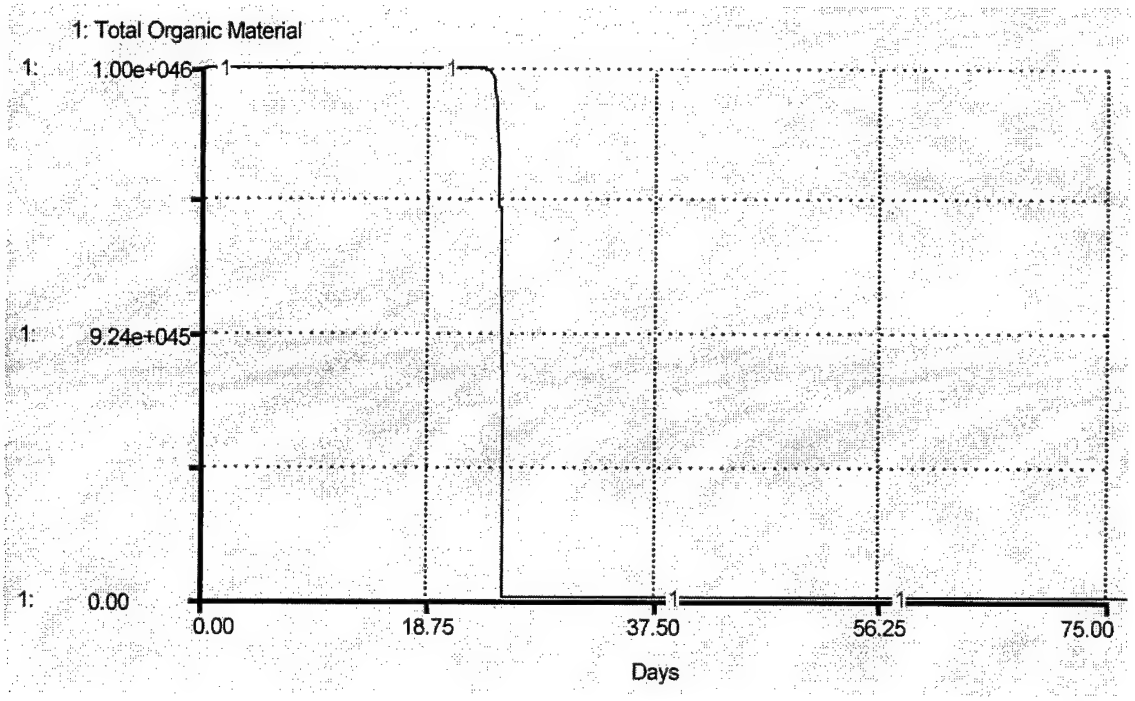


Figure 42. Anomalous Behavior Resulting from Altered Maximum Growth Rates

Not only does the output suggest much smaller values for maximum specific growth rates, but the experimental nature of the data for the per-day values also affirms the decision to use lower values. The values from experiments are under very controlled conditions and do not reflect the less than ideal nature of actual degradation sites.

Behavior Sensitivity

The final area of appropriate testing for the model centers on the sensitivity of the model to changes in its parameters. Do plausible changes in parameter values cause model failure? What effect do these changes have on model behavior? This type of testing merely involves altering parameter values and witnessing the results of the changes. The environmental parameters of moisture content and temperature will be analyzed, as well as the biokinetic constants of the Monod equations. These parameters are chosen because they offer the most likely avenues of change for the real system.

As in extreme condition testing, where similar structural representations exist in the model, one typical set of bacteria and its related phenomenon are chosen for each graph to simplify graphical presentation of the test results. Also note that such environmental parameter changes affect *every* bacterial group, and the sensitivity testing for each environmental parameter is a reflection of the combined effect on all groups for the parameter. As in other graphical presentations in this chapter, the scaling of each graph may be changed to enhance the output readability and the clarity of discussion regarding the model behavior being tested.

pH offers an avenue of change in the real system, but the changes resulting from pH are centered on the extreme condition values previously tested. Inside the optimal range for pH, there is little inhibitory influence from pH on the methanogenic system. Therefore, sensitivity testing involving the pH parameter was essentially discussed and tested earlier in the Extreme Testing section and will not be pursued further in this section. However, as some authors have noted, pH may indeed have unknown influence

on the other bacterial groups of the process (Al-Ghusain and Hao, 1995:234-235; Kasali and others, 1988:238). Such alternate influences are left for future efforts for understanding biodegradation and improving this modeling effort.

Moisture Content. The extreme condition testing of this parameter revealed expected system behavioral results when dealing with the possible extremes of moisture. Yet, what offers even more insight into the strength of this environmental parameter's influence rests with how sensitive the model is to moisture level changes within those extreme values. Fermentative bacteria and carbon dioxide generation are utilized as the representative entities for analyzing model behavior sensitivity to moisture content.

Figures 43 and 44 demonstrate the effects of increasing moisture content. The traces represent the following initial moisture levels: trace 1 is 20% moisture content; trace 2 is 40%; trace 3 is 60%; trace 4 is 80%; and trace 5 is 90% moisture content.

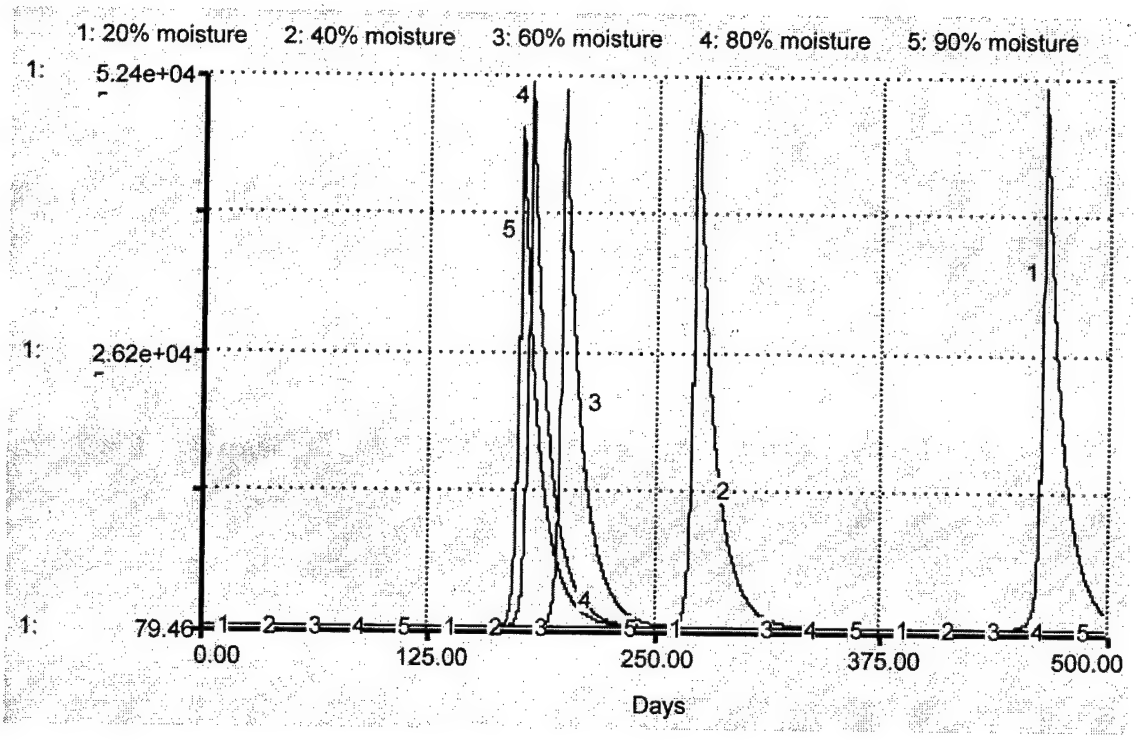


Figure 43. Bacteria Sensitivity to Changes in Initial Moisture Levels

As Figure 43 shows, bacterial growth happens much sooner when initial moisture levels increase. But this time differential shrinks as saturation is approached suggesting that once favorable moisture levels are reached the ability of moisture levels to continue to change to enhance bacterial growth diminishes. Figure 44, examining gas generation, confirms this result.

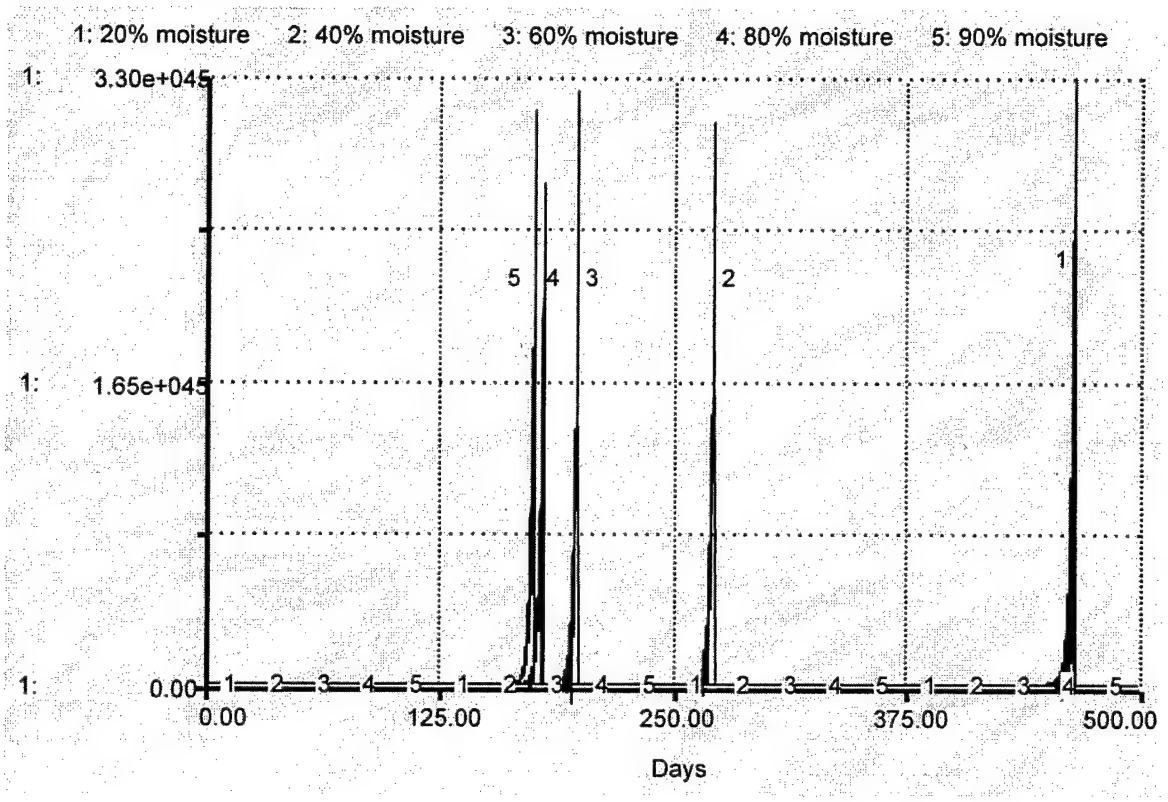


Figure 44. Gas Generation Sensitivity to Changes in Initial Moisture Levels

Degradation and subsequent gas generation are largely determined by bacterial growth, so the behavior in Figure 44 is consistent with that in Figure 43.

Temperature. Sensitivity testing for temperature involved changing the initial ambient temperature from 20 deg C to 35 deg C in 5 degree increments to analyze the effects of climbing temperature on model behavior. Traces 1 through 5 in Figures 45 and 46 represent the effects of 20, 25, 30, and 35 deg C temperatures, respectively, on behavior. To represent behavioral changes, the representative entities of methanogens and methane generation are utilized.

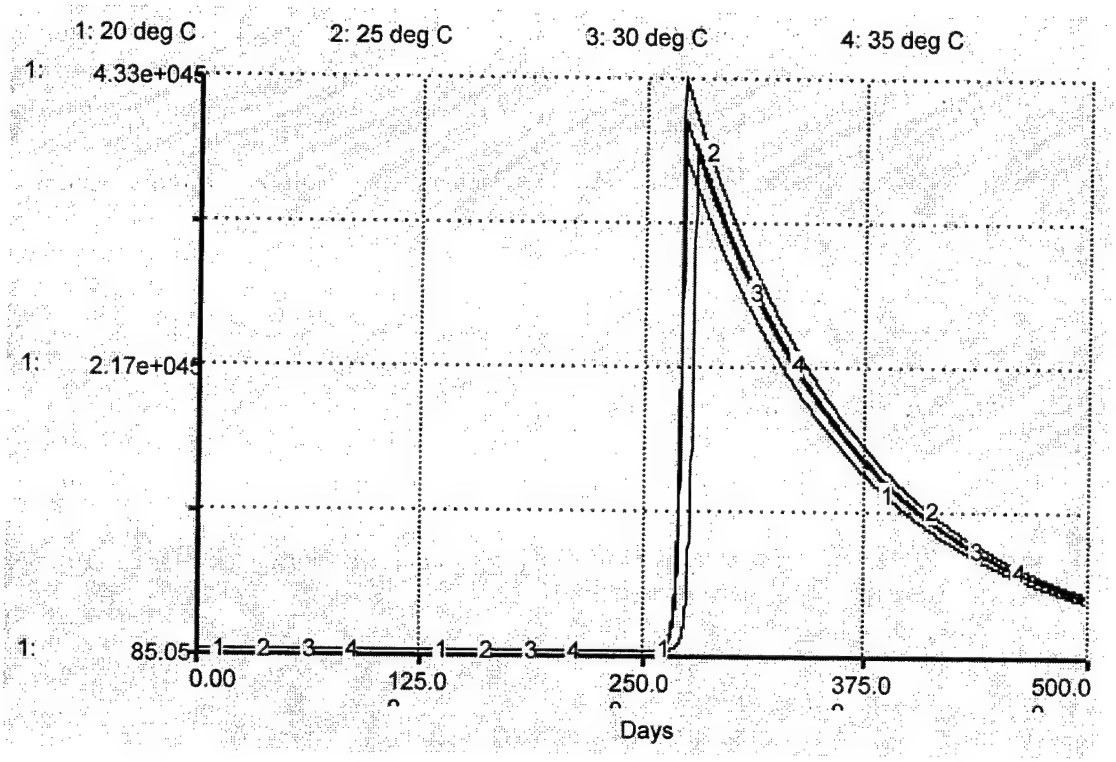


Figure 45. Bacteria Sensitivity to Changes in Temperature

Figure 45 illustrates the limited effect of altering the initial temperature conditions on bacterial growth. In the 20 to 30 degree range, there is no significant change in the timeliness or rate of methanogenic growth. At 35 degrees, the bacterial growth behavior is relatively unchanged. Figure 46 demonstrates that for gas generation behavior, the result is similar to Figure 45 regarding the sensitivity of model behavior to changes in temperature.

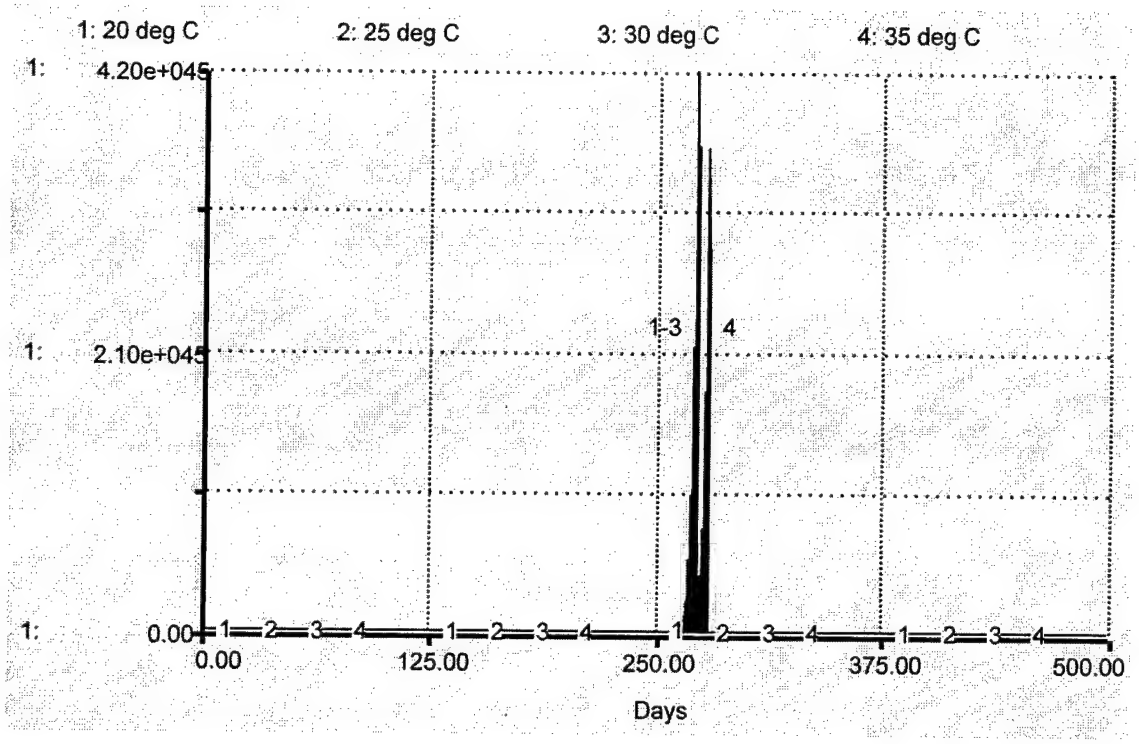


Figure 46. Gas Generation Sensitivity to Changes in Temperature

Monod Kinetic Parameters. The maximum growth rate and half saturation constant parameters determine the bacterial growth for the model. By testing behavior sensitivity to these parameters, one can see how bacterial growth for each group of bacteria affects the overall process. For these tests, each group's set of parameters were changed separately.

Maximum Growth Rate. The maximum growth rate for each bacterial group was changed by a plausible degree below and above the preset ("typical") model values. To gauge the effect of the alteration, bacteria and/or methane generation are utilized to represent the results. Methane generation is used because it is one of the final steps of the degradative process, allowing the alteration's ultimate effect on the process to

be viewed. Scaling for the graphs is often changed to enhance the presentation of the behavior being addressed.

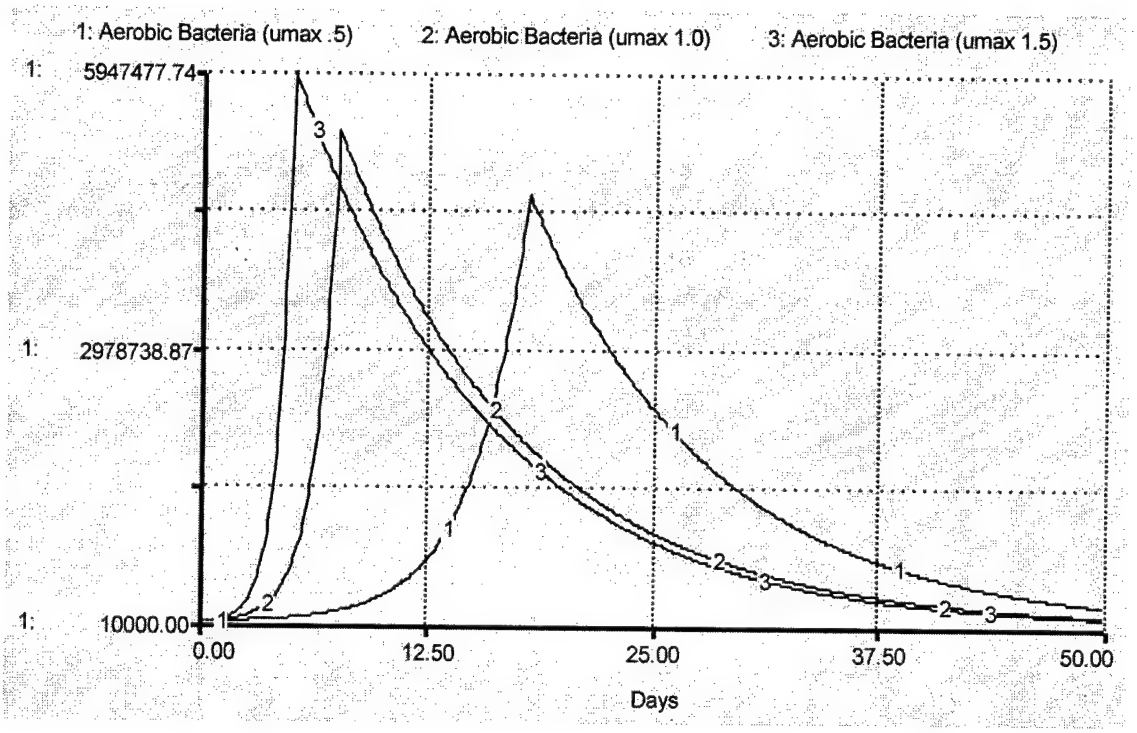


Figure 47. Sensitivity of Aerobes to Changes in Aerobic Maximum Growth Rate

As expected, as the maximum growth rate for aerobes changes from 0.5 (trace 1) to 1.5/day (trace 3), aerobic bacterial growth occurs both sooner and at a higher peak rate. Trace 2 represents the baseline rate of 1.0. Yet, the overall behavior pattern remains similar: exponential increase with a sudden drop to zero.

The next maximum growth rate tested belongs to the hydrolytic group of bacteria. Again the maximum rate was altered below and above the current model value. Trace 1, 2, and 3 represent behavior based on a rates of 0.25, 0.5, and 0.75/day respectively.

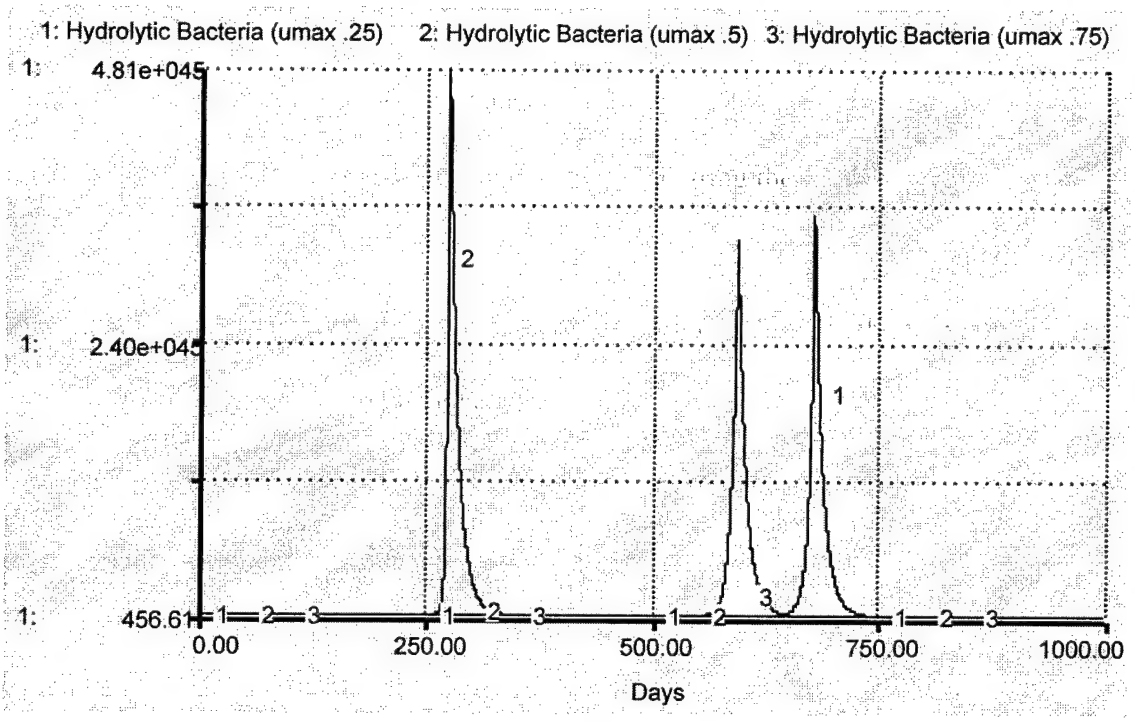


Figure 48. Sensitivity of Hydrolytic Bacteria to Changes in Maximum Growth Rate

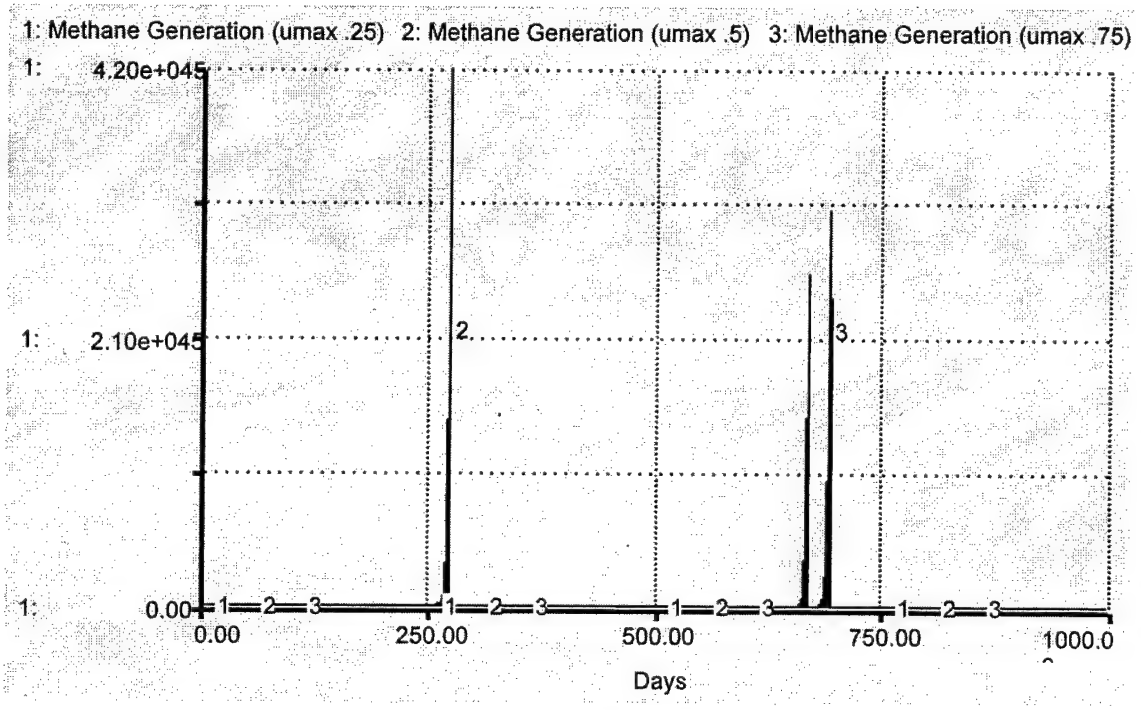


Figure 49. Sensitivity of Methane Generation to Maximum Hydrolytic Growth Rate

Figures 48 and 49 both demonstrate the sensitivity of model behavior to changes in the hydrolytic maximum growth rate. As the maximum rate is increased, bacterial growth increases, but notice that trace 3 is delayed even though it represents the greatest maximum rate. This phenomenon can be traced back to the inhibitory nature of higher temperatures.

Investigation reveals that the increased maximum growth rate eventually causes inhibitory temperature levels for the system because the increased growth rate is tied to microbial activity which influences temperature changes. Even though the hydrolytic bacterial growth is the only set of bacteria initially affected by the maximum rate change, its microbial activity ultimately affects the other bacteria groups by inducing a greater temperature change. The amount of methane generation also confirms this result with the highest maximum growth rate yielding a lower peak in methane generation. These results suggest that the relationship between microbial activity and temperature should be differentiated to better reflect the actual contributions of each bacterial group to temperature changes in the system.

Also note that in Figure 49, the lowest maximum growth rate results in negligible methane generation (as represented by trace 1) relative to the other traces. This behavior stems from the interdependency of methanogens on the preceding bacterial groups. Even though the lowest maximum growth rate for hydrolytic bacteria still results in hydrolytic growth, the growth is delayed enough to significantly delay the entire degradation process. The delay suppresses the growth of methanogens and subsequent methane generation (at least beyond the time frame presented) because the methanogens ultimately

depend on the hydrolytic bacteria to supply the necessary substrates to the bacteria which provide the methanogens with their required substrate.

Fermentative bacteria were examined third. Their maximum growth rate was changed from 0.35 to 0.85, with traces 1, 2, and 3 representing 0.35, 0.6, and 0.85/day, respectively.

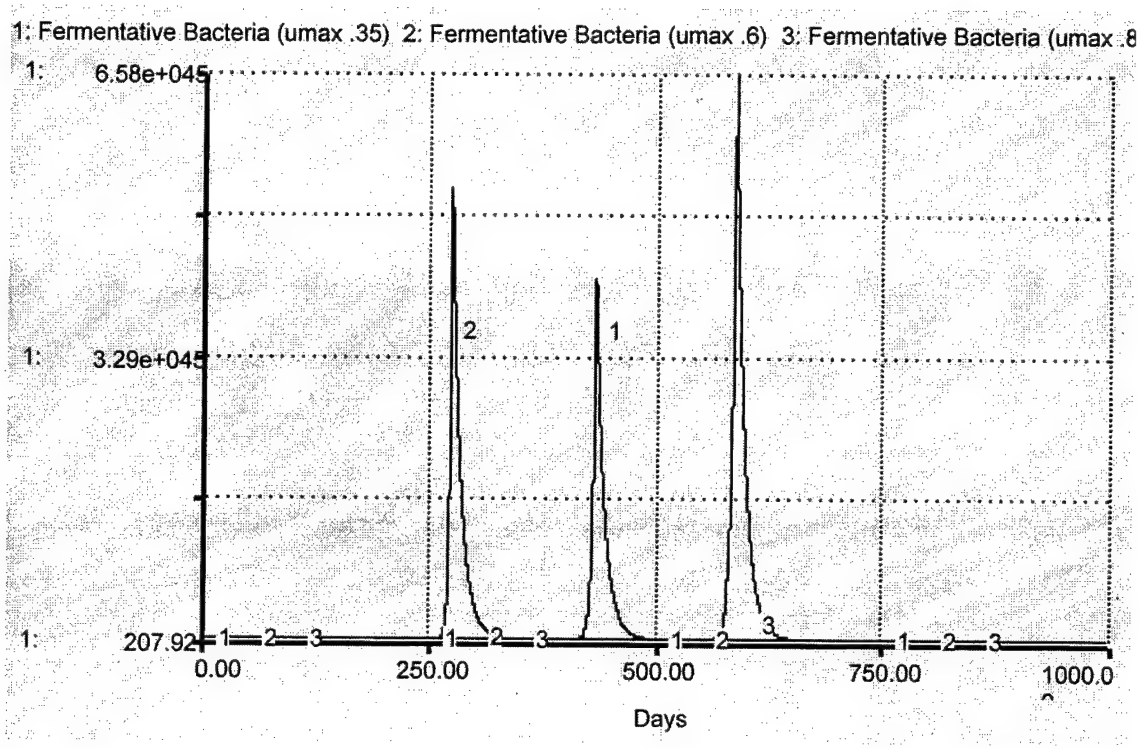


Figure 50. Sensitivity of Fermentative Bacteria to Changes in Maximum Growth Rate

Figures 50 and 51 demonstrate that altering the maximum growth rate for the fermentative group of bacteria results in increases in bacterial mass levels. However, similar to the model behavior concerning hydrolytic bacteria and methane generation, trace 3 experiences a delay. As with hydrolytic bacteria testing the amount of methane generation confirms this result; the highest maximum growth rate results in a delay in

methane generation. But the highest maximum growth rate change invokes a greater response in behavior than the previous anaerobic bacteria. Is this due to the higher rate offering even greater inhibitory temperature levels? Testing the remaining anaerobic bacteria should reveal the answer. Also, note the lowest maximum growth rate does not result in negligible relative methane generation as in Figure 49 since the fermentation step of degradation is "closer" to methanogenesis than hydrolysis.

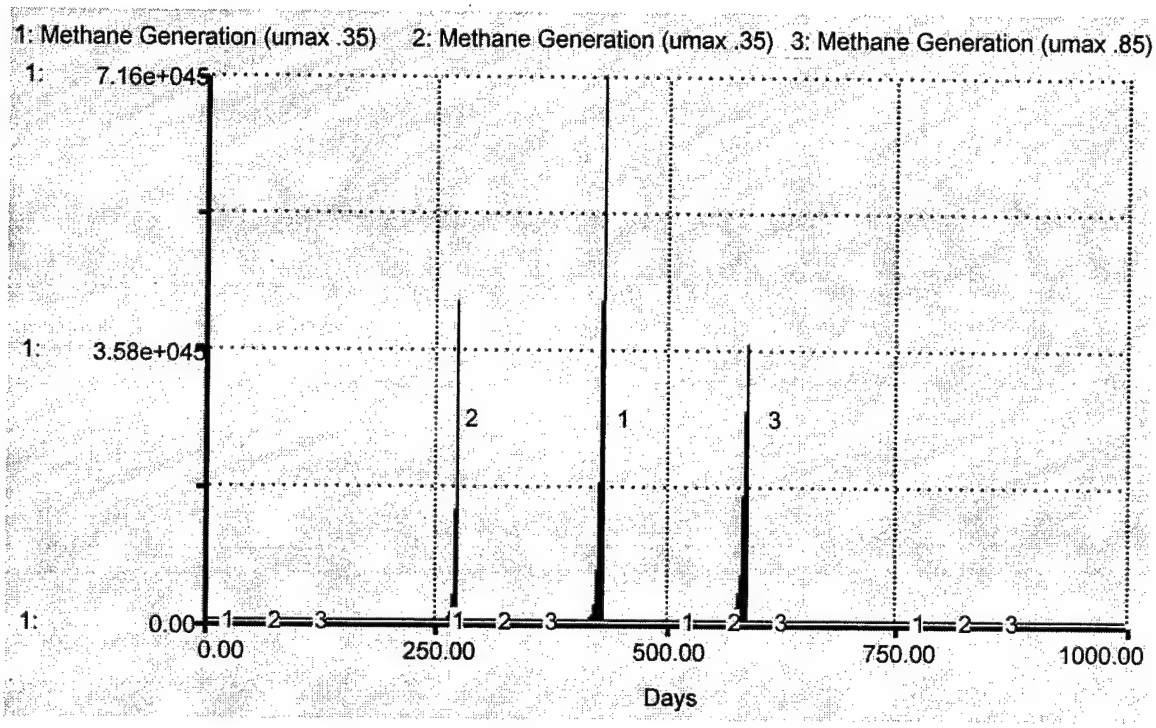


Figure 51. Sensitivity of Methane Generation to Maximum Fermentative Growth Rate

Finally, the acetogenic and methanogenic maximum growth rates are examined separately. Traces 1, 2, and 3 of Figures 52 and 53 represent maximum growth rates of 0.30, 0.55, and 0.80, respectively, for the acetogenic bacteria, while traces 1, 2, and ,3 of Figures 53 and 54 depict rates of 0.275, 0.525, and 0.775 for the methanogens.

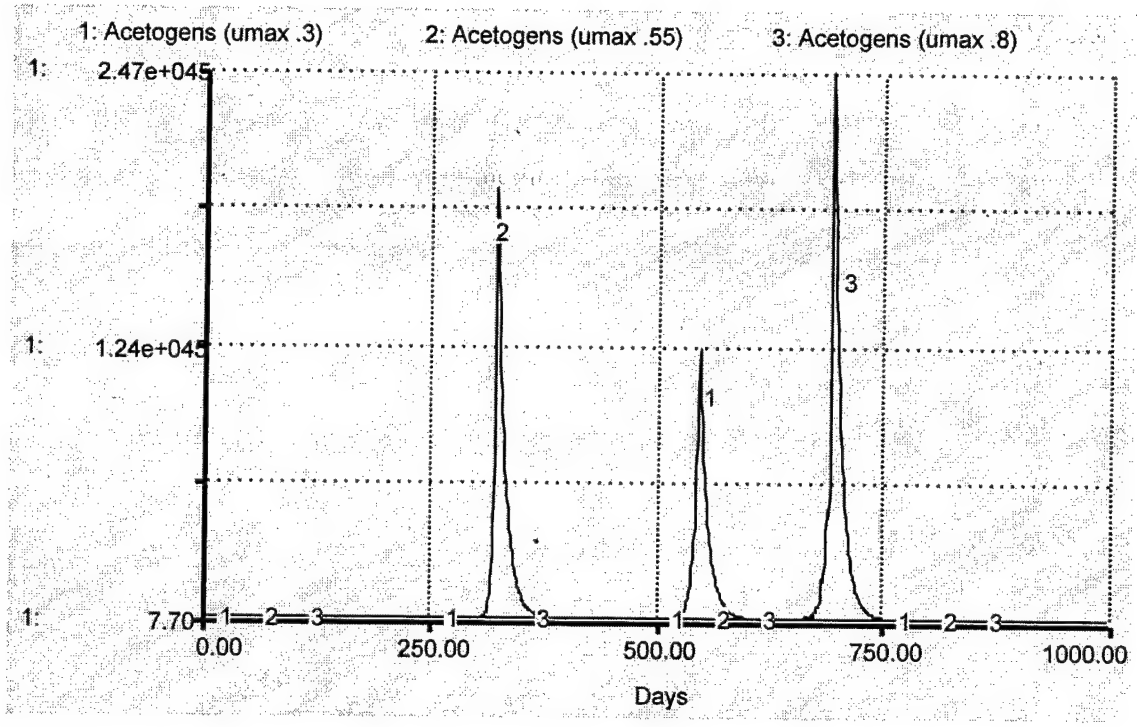


Figure 52. Sensitivity of Acetogens to Changes in Maximum Growth Rate

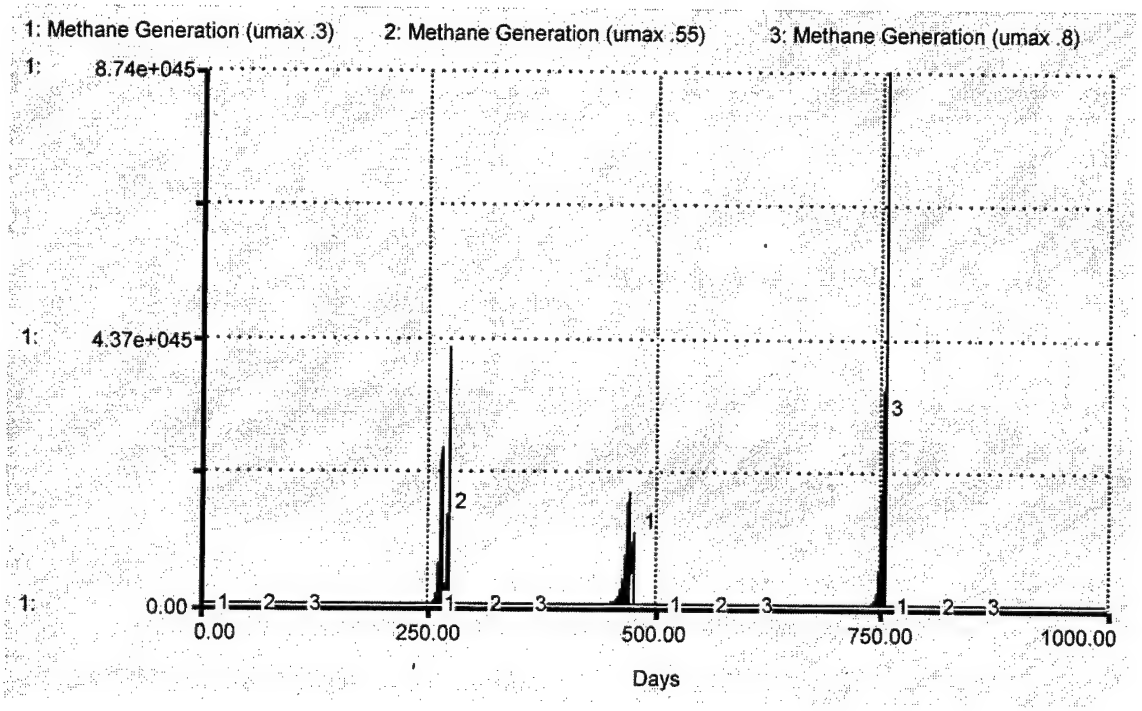


Figure 53. Sensitivity of Methane Generation to Maximum Acetogen Growth Rate

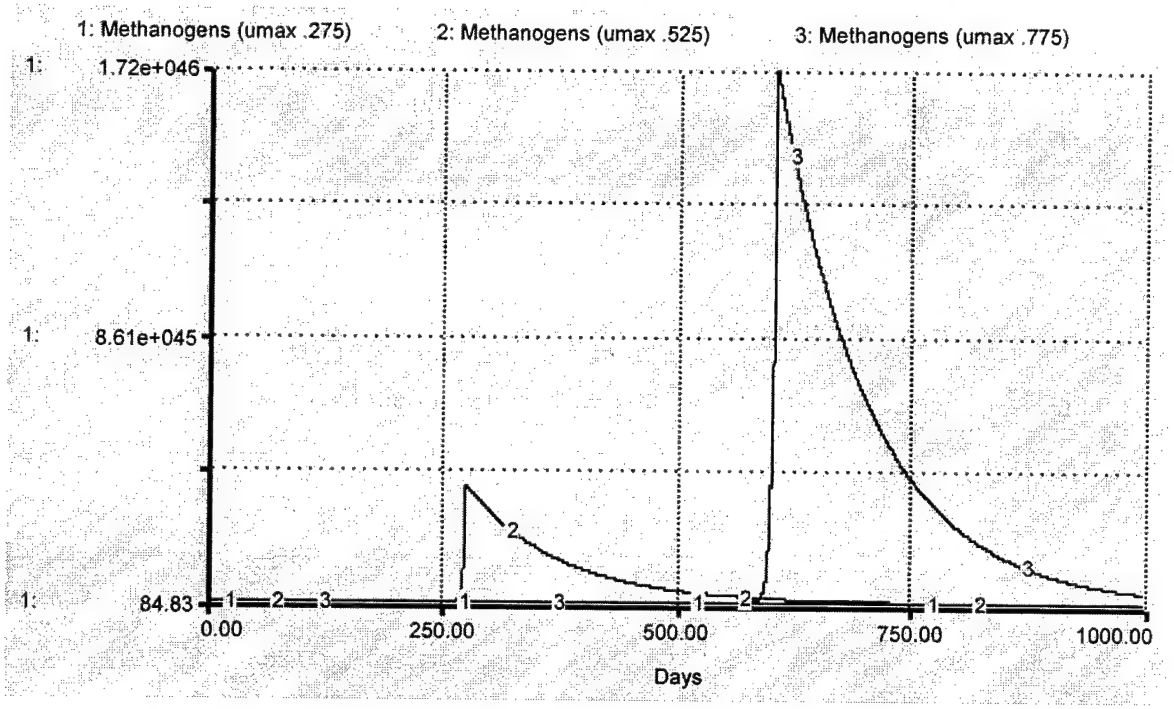


Figure 54. Sensitivity of Methanogens to Changes in Maximum Growth Rate

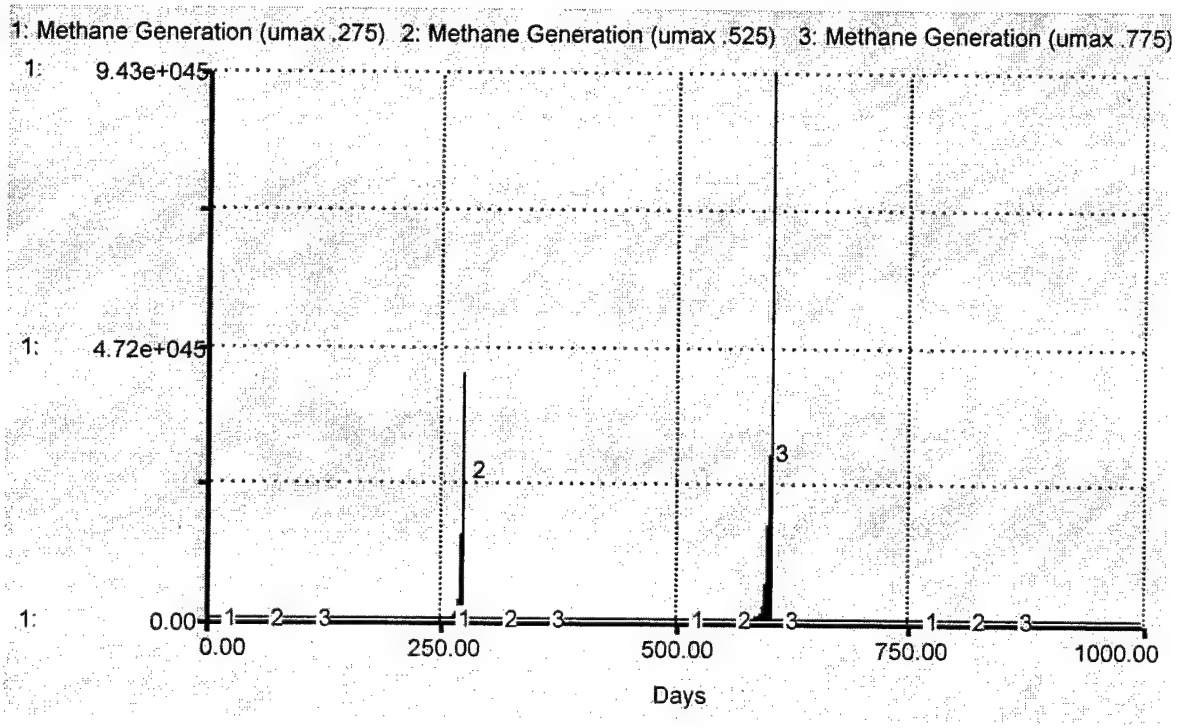


Figure 55. Sensitivity of Methane Generation to Maximum Methanogen Growth Rate

As with the hydrolytic and fermentative bacteria testing, altering the maximum growth rates to the highest maximum growth rate tested for the bacteria results in methane generation being delayed. The same phenomenon regarding delayed methane generation with the highest maximum growth rate as witnessed with the other anaerobic bacteria is present when testing with acetogens and methanogens. However, the peaks for methane generation associated with the highest maximum growth rates are now much higher than the methane generation corresponding to the lower maximum growth rates tested (in contrast to the previous anaerobic bacteria).

This behavior appears to stem from not only the inhibitory temperatures mentioned previously, but also the wait involved for these bacteria in obtaining the necessary substrate for energy and the close association between acetogens and methanogens. As these bacteria wait for their particular substrate to be available, the other bacteria are changing the environmental conditions even before the acetogens and methanogens have a chance to affect their environment themselves. Since bacterial growth ultimately determines substrate utilization and subsequent gas generation, methane generation also exhibits the same general type of behavior. Since acetogens are in direct contact with methanogens providing them with the necessary substrates for energy, it seems logical any change in acetogenic growth rates would have a greater effect on methane generation. Obviously, any alteration to methanogen growth rates will have a significant impact on methane generation as long as the conditions necessary for methanogen survival are met.

Examination of the sensitivity of the model to bacterial growth and gas generation is clearly helpful in understanding the intricacies of the effects of maximum growth rate on the model. Yet, viewing the big picture while conducting sensitivity testing may also build confidence in the model. For example, increasing the maximum growth rate of the acetogens should increase the percentage of hydrogen gas in the system.

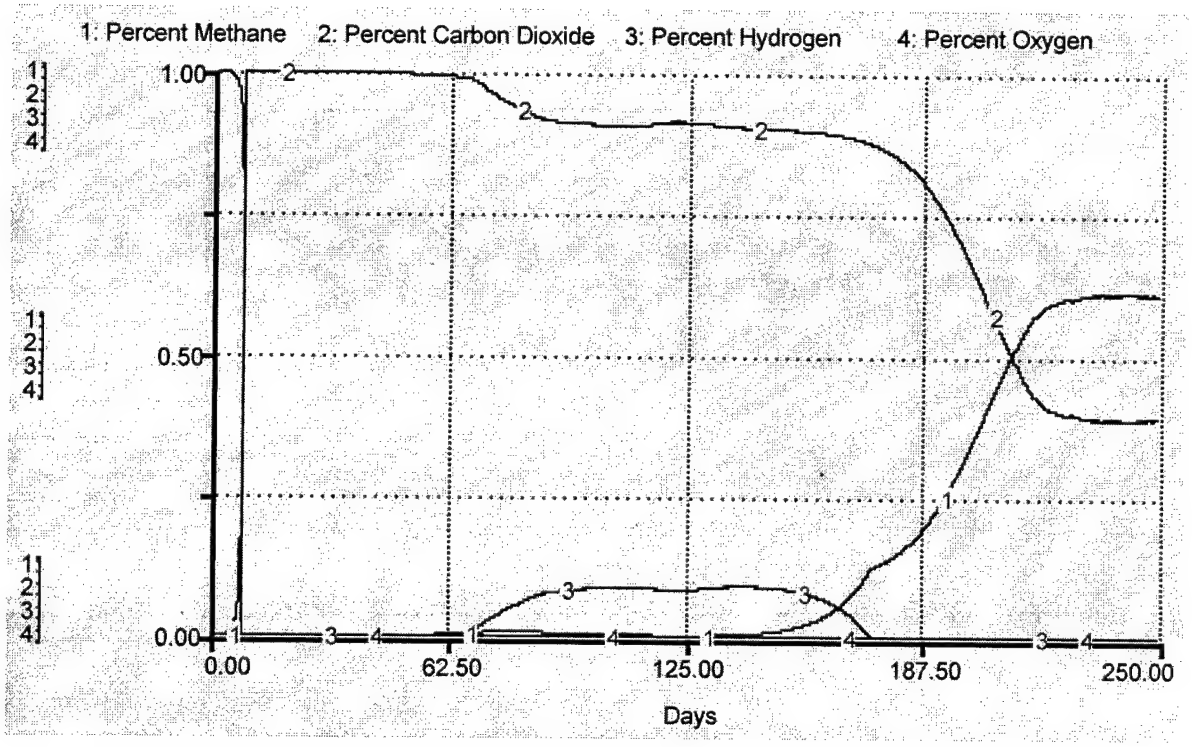


Figure 56. Sensitivity of Model Behavior to Maximum Acetogen Growth Rate

As Figure 56 demonstrates (when compared to Figure 16), the percentage of hydrogen gas does increase as the maximum acetogen growth rate increases to 0.80. Moreover, it illustrates the inhibitory behavior discussed previously by delaying methane gas production. This inhibitory behavior can also be seen in Figure 57 (when compared to Figure 16), where methane gas production (as depicted by percent composition within

the system) is again delayed as the maximum fermentative growth rate is increased from the baseline of 0.6 to 0.80.

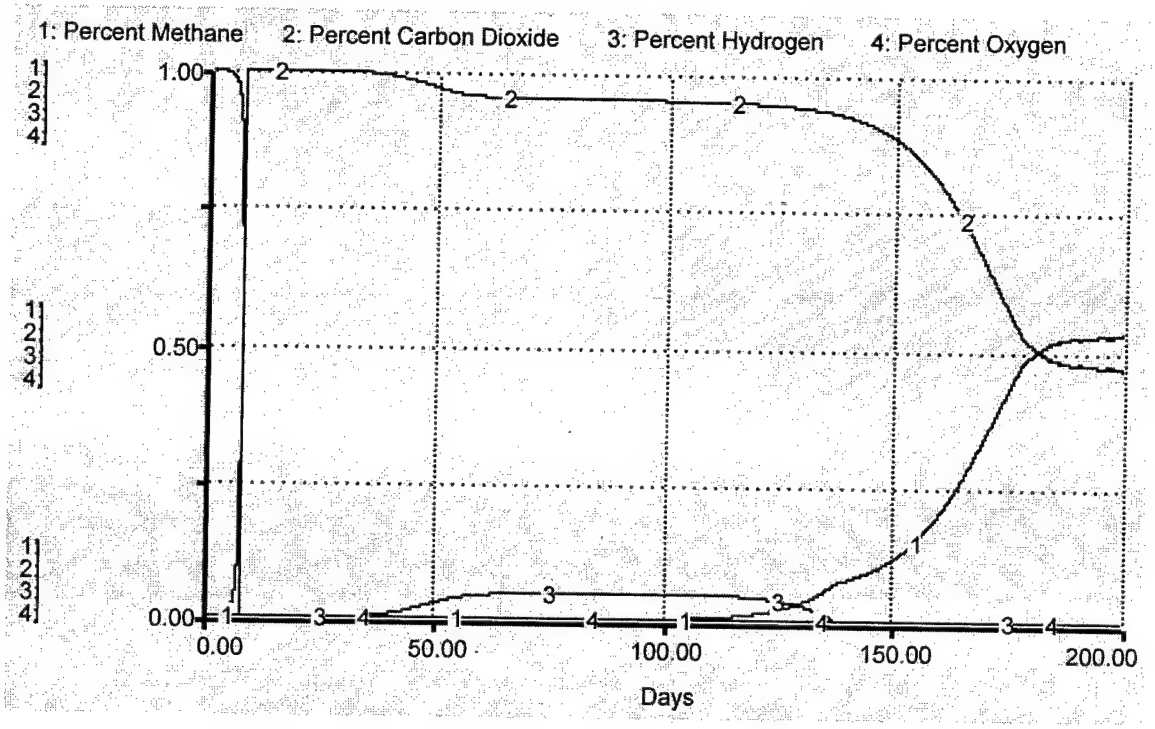


Figure 57. Sensitivity of Model Behavior to Maximum Fermentative Growth Rate

These "big-picture" graphs not only affirm the behavior seen in the other sensitivity outputs but also build confidence in the model overall as plausible behavior is witnessed through sensitivity testing.

Half Saturation Constant. The half saturation constant for each bacterial group was changed by orders of magnitude above the baseline (or "typical") values. To gauge the effect of the alteration, bacteria and methane generation are utilized to represent the results. Methane generation is used for the same reasons stated for maximum growth rate sensitivity testing: methane generation is used because it is one of the final steps of

the degradative process, allowing the alteration's ultimate effect on the process to be viewed. Proper scaling was applied where necessary to enhance analysis of model behavior.

Before bacterial growth and gas generation outputs were viewed, the half saturation constant was changed to ensure the half saturation constant is modeled correctly with regards to Monod kinetics. If modeled correctly, altering the constant should change the shape of the growth rate curve based on the Monod equation for bacterial growth.

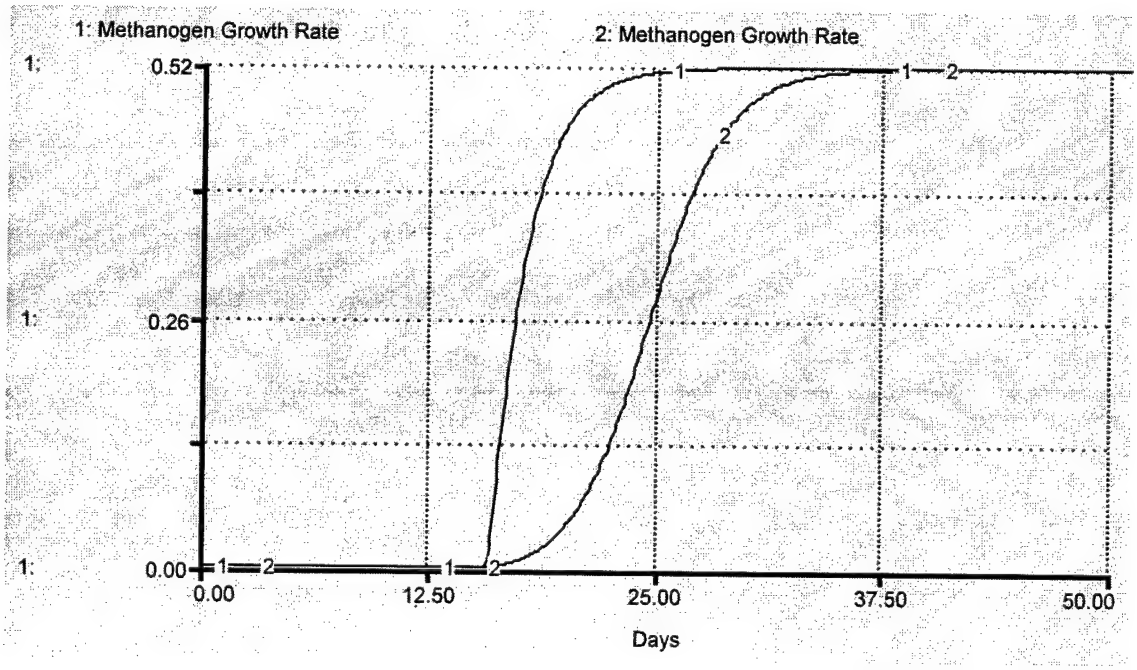


Figure 58. Effect of Changing Half Saturation Constant on Growth Rate

Figure 58 clearly shows that changing the half saturation constant does indeed change the shape of the growth rate curve consistent with Monod kinetics.

Beginning with the aerobic bacteria, it is evident that changing the half saturation constant for the aerobic bacteria does not significantly change model behavior until a much larger parameter value is utilized. Trace 1 and 2 follow the same behavioral pattern, and only when the half saturation constant grows significantly larger does it have an effect on behavior. (For all graphs concerning the half saturation constant, traces 1, 2, and 3 represent the baseline constant for the bacteria, 1 x 10^{20}, and 1 x 10^{45} mg, respectively.) Clearly aerobic growth is slightly delayed as the half saturation constant is increased due to the resultant smaller growth rate.

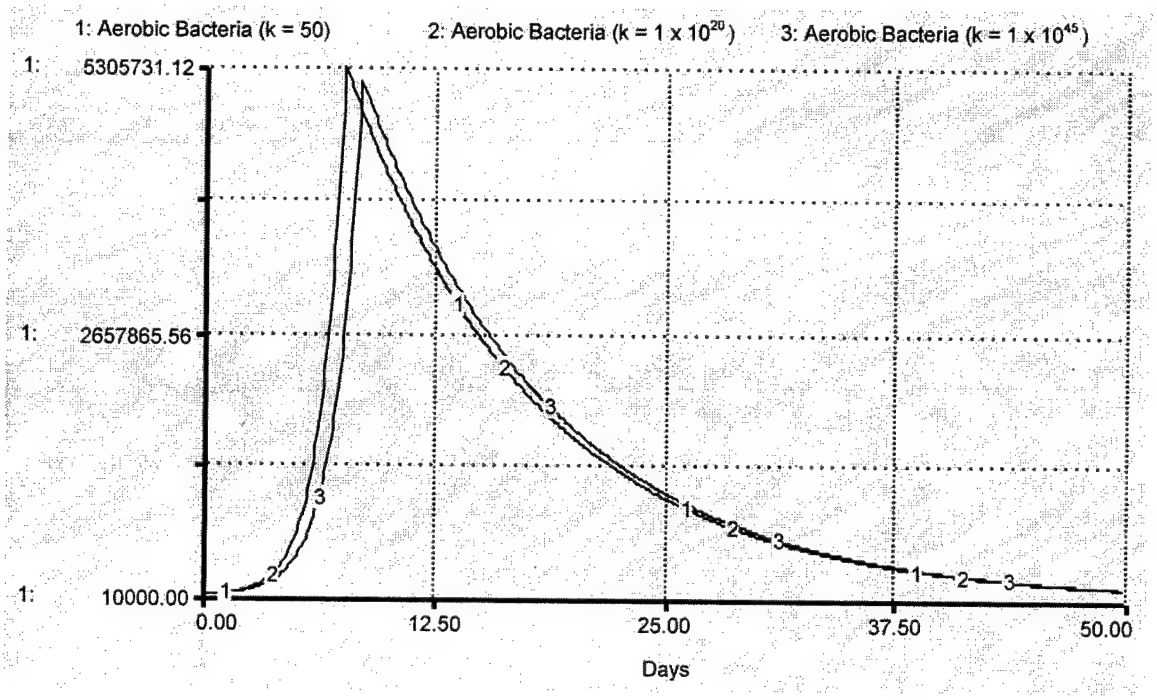


Figure 59. Sensitivity of Aerobic Bacteria to Aerobic Half Saturation Constant

For the anaerobic stages, it was discovered that model behavior demonstrates greater changes as the half saturation constants are changed further down the progression of degradation. In other words, changing the half saturation constant for methanogens

invokes a greater change in model behavior than does altering the hydrolytic bacteria half saturation constant. Figures 60 through 67 illustrate bacteria and methane generation behavior as the half saturation constants are changed for each set of anaerobic bacteria.

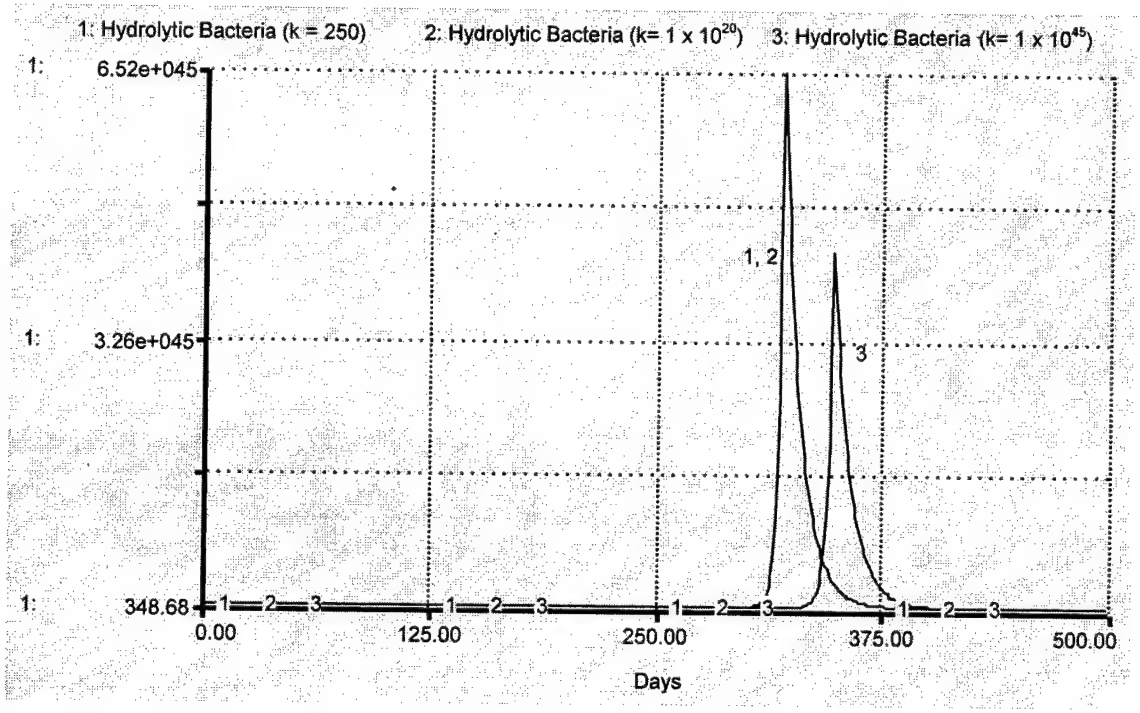


Figure 60. Sensitivity of Hydrolytic Bacteria to Hydrolytic Half Saturation Constant

For the hydrolytic bacteria, the resultant behavior is quite similar to the aerobic bacteria where it requires a much larger half saturation constant to alter bacteria behavior. Methane generation in Figure 61 illustrates corresponding behavior; less hydrolytic bacteria ultimately means less substrate being funneled through the degradation process which explains trace 3 of Figure 61.

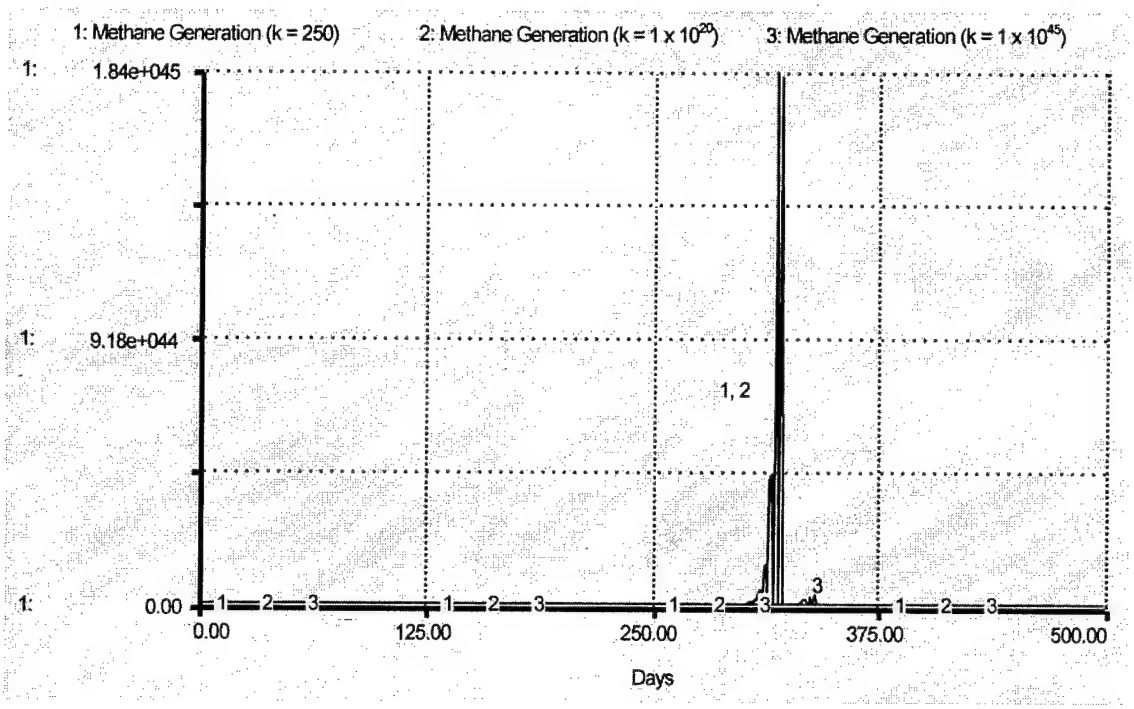


Figure 61. Sensitivity of Methane Generation to Hydrolytic Half Saturation Constant

Remembering that hydrolytic bacteria do not have to "wait" for their substrate to be provided, the other anaerobic bacteria may be more sensitive to changes in their half saturation constant. As their constant increases, it slows their growth, limiting their ability to convert substrate into useable products for the follow-on degradative step.

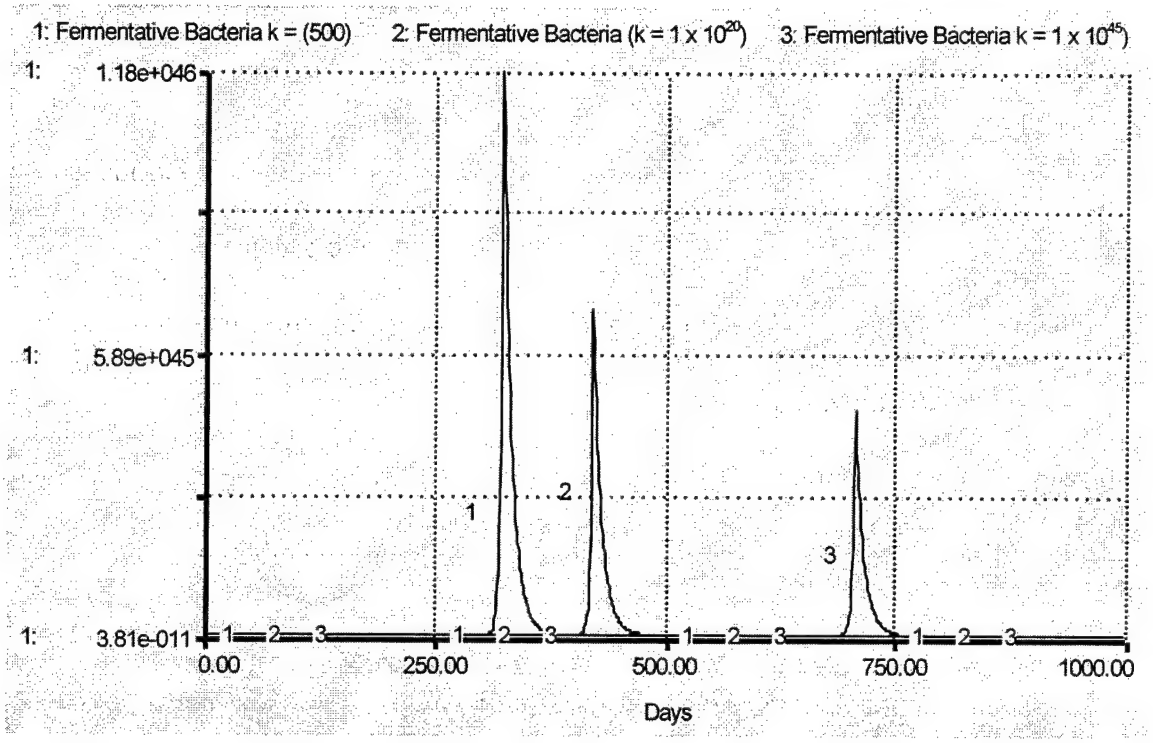


Figure 62. Sensitivity of Fermentative Bacteria to Fermentative Half Saturation Constant

As Figures 62 and 63 illustrate, the fermentative bacteria are more sensitive to changes in their half saturation constant than the hydrolytic bacteria. Unlike the hydrolytic bacteria, fermentative bacteria must have their substrate provided by a preceding group of bacteria. An increasing half saturation constant slows their growth causing an expected decrease in their mass. Methane generation behavior in Figure 63 is comparable to the bacterial behavior of Figure 62. Such behavior should be seen in the remaining anaerobic bacteria of the degradation process.

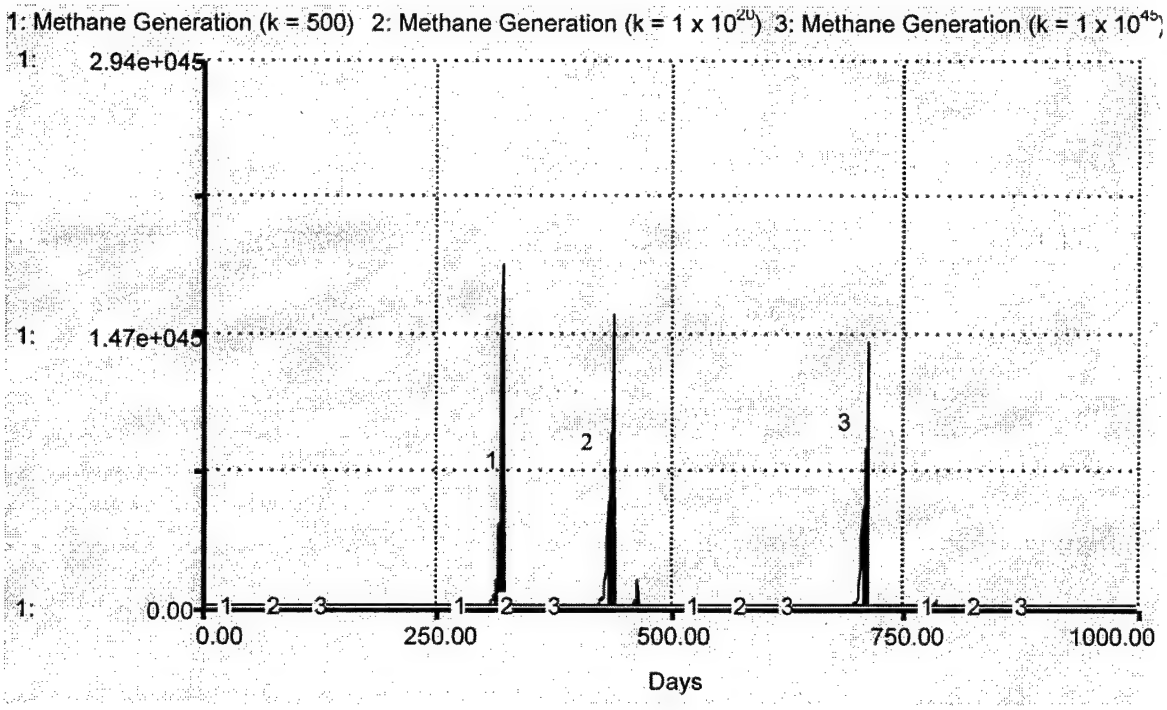


Figure 63. Sensitivity of Methane Generation to Fermentative Half Saturation Constant

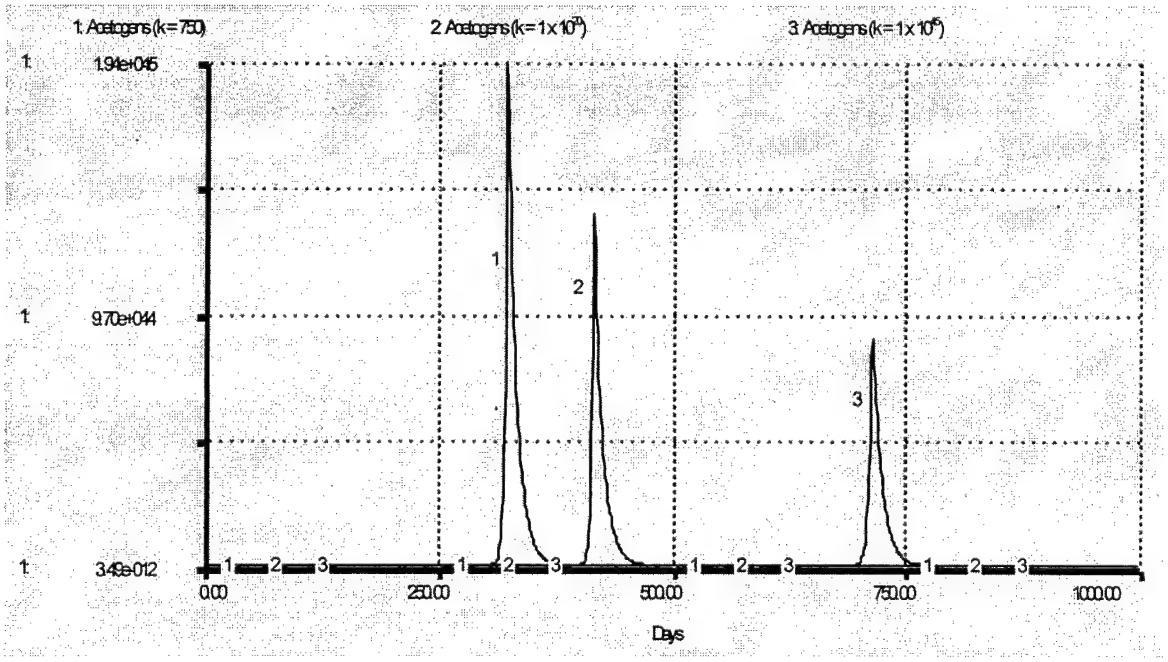


Figure 64. Sensitivity of Acetogens to Acetogen Half Saturation Constant

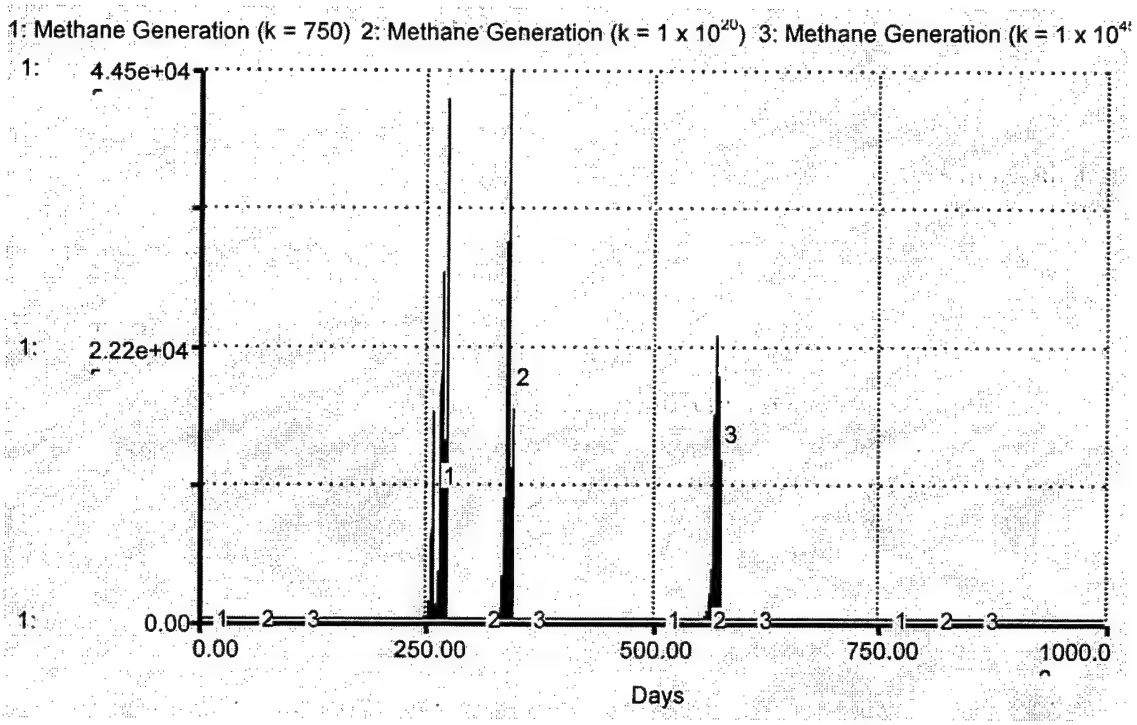


Figure 65. Sensitivity of Methane Generation to Acetogen Half Saturation Constant

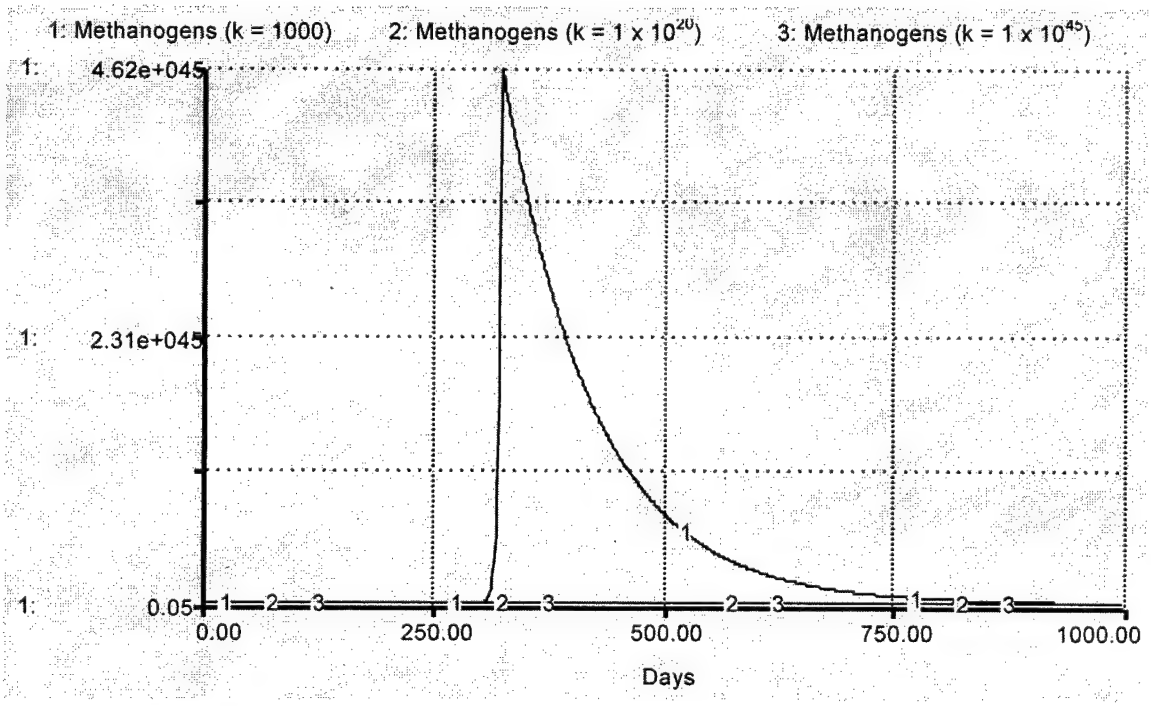


Figure 66. Sensitivity of Methanogens to Methanogen Half Saturation Constant

For the methanogens, the behavior resulting from changes in its half saturation constant seems quite significant. Although trace 1 for Figures 66 and 67 is the only one visible, the other traces exist. The relative magnitude of trace 1 masks the other two traces. The important point made by both the figures centers on the methanogens dependency on the preceding degradative steps. When slower growth is induced with higher half saturation constants, the methanogens and methane generation are greatly reduced because methanogens must naturally wait for the preceding degradative steps to occur before their required substrate becomes available.

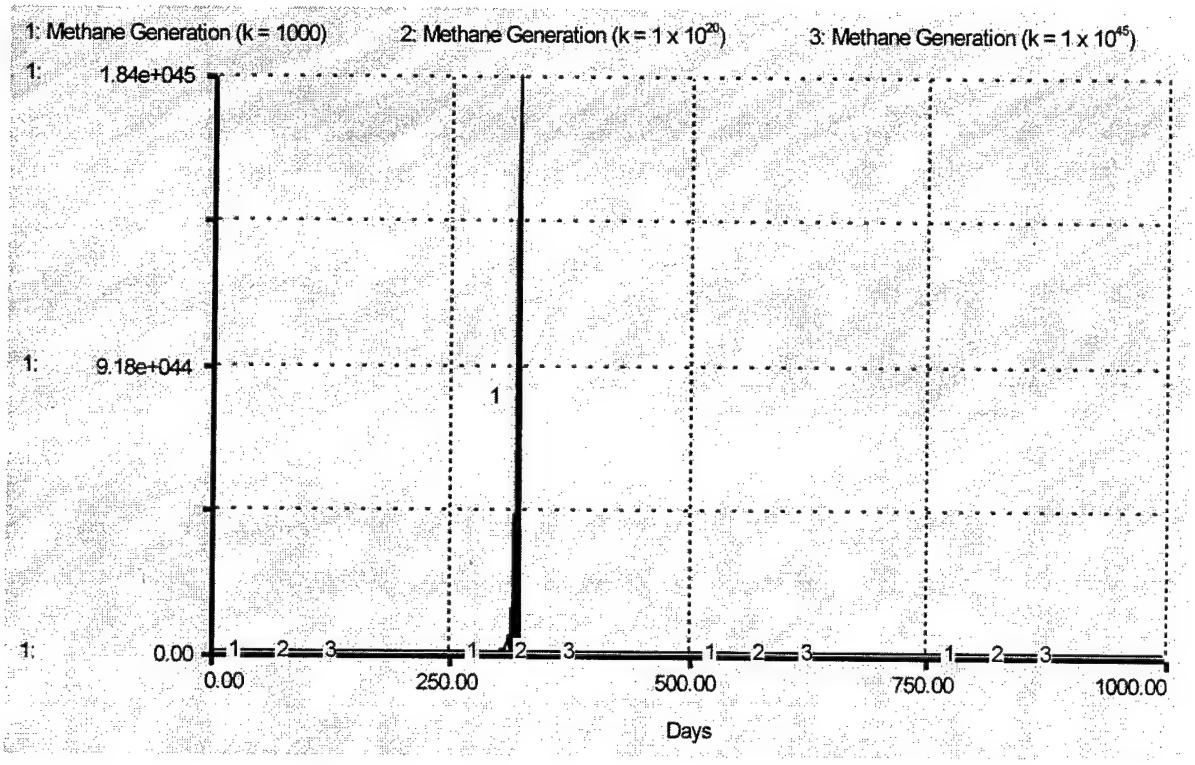


Figure 67. Sensitivity of Methane Generation to Methanogen Half Saturation Constant

In general, higher half saturation constants for each set of bacteria do lead to expected reductions and delays in bacterial peaks and methane generation, but the effect

becomes more pronounced as the constant is changed for bacteria further in the degradation chain. Altering the constant does not appreciably change the behavior of model entities with regard to shape of the resultant plots. The half saturation constant does have to be changed to a significantly larger value for the behavior to be altered, but this should be somewhat expected given the large amounts of substrate found in the model. Such large values for the half saturation constant differ greatly from those determined with parameter verification (see Parameter Verification section). Due to the uncertainty surrounding the numerical accuracy of this entity the larger values are utilized for sensitivity testing to illustrate the influence half saturation constants can have in determining the state of the system given its effects on bacterial growth.

Conclusion

While numerous confidence tests exist for system dynamics models, one must choose the appropriate tests in order to facilitate efforts in building confidence in a model's ability to represent the real world and simulate actual processes. The tests utilized for this thesis effort are the most applicable (concerning the nature of this system and model) in generating confidence for the constructed model. For example, tests for policy implications test the effects of altering different policies on the model behavior, but the current model does not address landfill managing policies. Moreover, the entities analyzed during the testing were chosen for their appropriateness for the particular test; other entities were ignored (such as the stoichiometric ratios for each degradative step) because their values are based on concrete scientific methods with little chance for realistic fluctuation given the current model assumptions.

Overall, the confidence testing performed revealed the complexity of representing a system where behavior is often defined by more than one interaction between entities and the difficulty of pinpointing the cause of such behavior. Each step of the degradative process can influence another, directly or indirectly. Reasonable confidence can be assumed in the model's ability to represent the progression of the biodegradation process and to establish the basic interrelationships between bacterial groups, substrates, and environmental conditions. However, little confidence is attained in certain areas of the model to include: the omission of substrate availability aspects of the system; the lack of completeness in representing the syntrophic relationship of acetogens and methanogens; and the simplicity of the functions employed to describe the relationship between bacteria and the environmental conditions. Unfortunately, the ability to portray the confidence (or lack of confidence) in the model and to discuss model behavior in greater detail was at times constrained by software limitations. These limitations centered on the capability of the software to import graphs that were altered in scale in order to better view the model behavior being addressed. Finally, it must be emphasized that as future efforts alter the structure and assumptions of the current model, testing must be reaccomplished to ensure the improved model is properly validated.

V. Conclusions and Recommendations for Further Study

Confidence in a model is built through validation and sensitivity testing. Such confidence is not only increased by witnessing expected plausible behavior throughout a range of parameter values, but also by identifying the limitations of the model in achieving its purpose. Through sensitivity testing, several conclusions regarding the biodegradation process and the influence of various parameters became apparent.

First, the parameters defining bacterial growth and environmental conditions are very interrelated. Changing a parameter associated with growth for even one set of bacteria can have lasting effects throughout the system. Such an alteration can eventually feed back to bacterial growth by redefining the environmental conditions for growth. For example, if fermentative bacterial growth increases relative to the other bacteria and lowers the pH level through increased acid production, the environmental condition of pH will be altered. This change in environmental condition eventually influences bacterial growth for other bacteria, especially methanogens.

Second, as one moves through the chain of degradative steps, the bacterial groups become more sensitive to changes in the system. The behavior of acetogens and methanogens of phases 3 and 4 is more dramatically altered by changes in system conditions than are the aerobic and hydrolytic bacteria prevalent in phases 1 and 2. Changes initiated in the earlier stages of the process seem to become magnified rather than dampened as the process continues into later stages.

Last, of the parameters tested, model behavior appears to be more sensitive to the environmental parameter of moisture content and the biokinetic parameter of maximum growth rate. Of course, within such a complex system, sensitivity to changes in the system may stem from not only the one parameter altered but also from the combination of effects brought about by the initial change. Such interrelated influences make it difficult to judge just how sensitive behavior is to the single parameter changed. For example, if the initial moisture content is rather high, it allows for increased bacterial growth leading to increased microbial activity which affects the temperature of the system. Thus, changes in behavior may not be from the influence of moisture content alone, but also the resultant effects moisture content has on the rest of the system.

Model Strengths

Given the model's purpose of simulating the fundamental processes of biodegradation within the landfill biochemical reactor, clearly the model succeeds in its ability to simulate the progression of degradation and establish an appropriate boundary for including the requisite entities needed to model the fundamental processes of landfill biodegradation. Moreover, it captures the interrelationships and feedback loops within and between steps. Thus, the model is able to verify the dependence each step and its associated bacterial group has on all other processes of the system. The model allows for simulation and testing of the various entities to evaluate system behavior, as well as validating the phenomena reported in literature.

With this model, the degradative steps of aerobic degradation, hydrolysis, fermentation, acetogenesis, and methanogenesis are reproduced. Corresponding to these

degradative steps, the landfill gases of oxygen, carbon dioxide, hydrogen, and methane can be observed. Lastly, the effects of influential environmental conditions (temperature, pH, and moisture content) are represented.

Model Limitations

As with any model, limitations exist. Although the current model produces plausible behavior commensurate with the reference mode, model validation pinpointed several weaknesses in the model. During the validation testing, several model weaknesses were identified which limit the model's ability to completely simulate the biodegradation of landfill disposal mechanistically. Clearly, the major limitation to be addressed is the mechanism associated with substrate availability. Not only will addressing this mechanism improve the mechanistic nature of the structure of the model, but should also eliminate the current model's anomalous behavior.

Another weakness derived from structural verification concerns the syntrophic relationship between acetogens and methanogens. While the current model allows for consumption of hydrogen by methanogens, it fails to limit the production of hydrogen gas by acetogens if such methanogenic consumption is reduced substantially for whatever reason. In other words, when less than optimal conditions exist for methanogens, one would expect hydrogen production to decrease or even cease accordingly. The current model only slows down hydrogen production based solely on the conditions affecting the acetogens. Obviously, under less than optimal conditions, processes involving acetogens and methanogens would be affected.

The use of a mass basis for the model, while simplifying the incorporation of several components into the model (such as stoichiometric ratios), made it more difficult to ascertain the plausibility of parameters associated with Monod kinetics and pH, which are normally addressed in terms of concentration. The use of concentration-based entities in the model may simplify the verification of parameters and sensitivity testing for certain parameters.

The simplistic nature of the representation of the relationship between system entities and the environmental parameters also limits the model's ability to completely address the effects of these parameters. The functions representing the parameter's influence on bacterial growth are solidly founded in the literature. The functions linking the environmental conditions such as temperature to system phenomena are generally mechanistic but simplistic in nature. Such simplicity is necessary in the absence of reliable theoretical or empirical data, and also makes it more difficult to establish a high level of confidence in the function's structure. For example, temperature changes are modeled as a function of microbial activity, which is tied to bacterial growth. This relationship is realistic and defensible but the degree of influence microbial activity actually has on temperature is not well understood.

Suggestions for Further Study

These weaknesses in the model detract from the model's utility as a management tool, at least in its present form, but they also suggest where researchers should look to answer important questions about the biodegradation system and offer particular avenues of exploration in improving the current model. Some of these questions are:

- What mechanisms are responsible for limiting substrate access?
- Does substrate access differ significantly for each class of bacteria?
- How strong is the syntrophic relationship between acetogens and methanogens, and what mechanism determines that strength?
- Do the different environmental conditions affect the various bacteria differently?

Such questions arising from the limitations discovered in the model, and the weaknesses themselves help to focus future efforts on improving the foundation this model has provided for examining the fundamental processes of the landfill as a biochemical reactor.

Certainly, the weaknesses of the current model need to be addressed in future efforts. Not only should the current weaknesses be addressed, but through further testing of the improved model, the basic approach may also be questioned. For example, although Monod kinetics is a classical approach to modeling bacterial growth and is essential to the current model, perhaps it does not fully address the relationship between substrate and bacteria in landfill conditions. Figure 68 illustrates model behavior when a graphical representation defines the substrate/bacterial growth relationship allowing for a more plausible initial substrate-to-bacteria ratio.

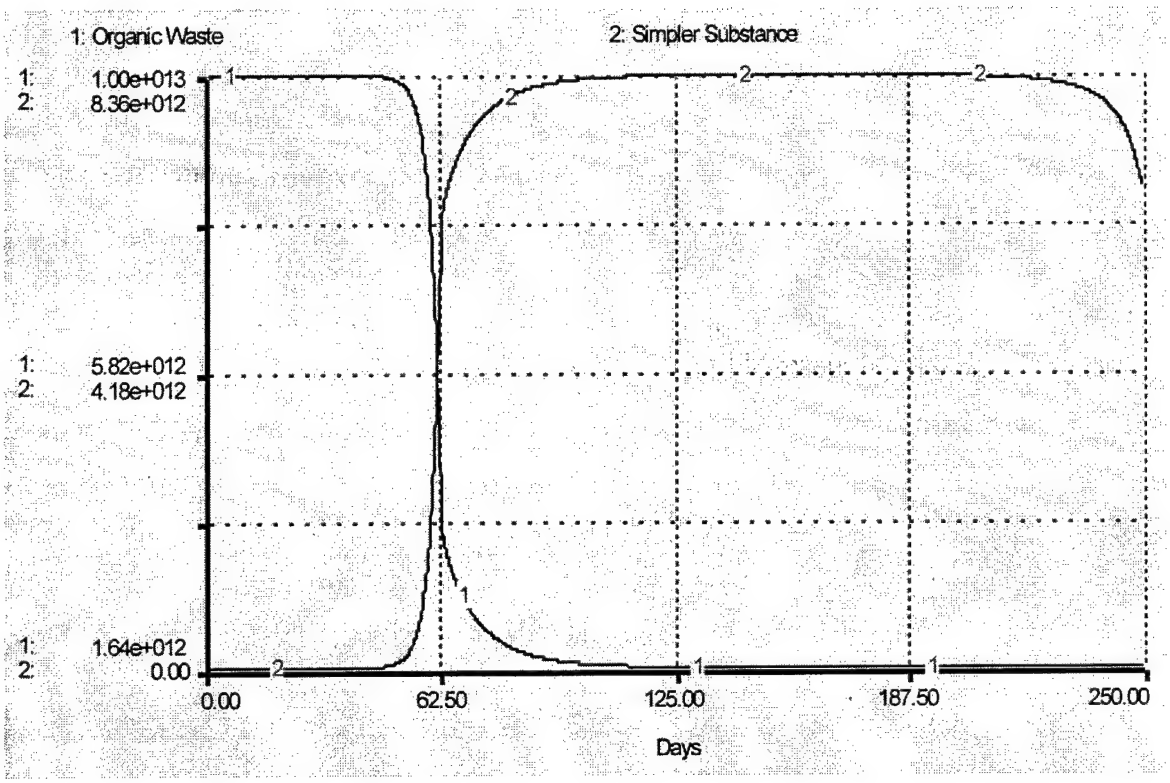


Figure 68. Substrate Utilization Employing Graphical Definitions of Bacterial Growth

Figure 68 demonstrates that by utilizing a graphical function to define substrate depletion instead of an equation derived from Monod kinetics (an equation the current model employs), organic material is not depleted in an unreasonably short period of time given the initial conditions of the model. Moreover, the initial organic material/bacteria ratio is more plausible than the current model ratio because the graphical function allows for a reduction in the value of the initial amount of organic material. However, employing a graphical function to define substrate depletion has no empirical or literature foundation. Therefore, Monod kinetics is utilized. The discussion is merely intended to emphasize that model structure itself can be questioned in the future and should not be instantly accepted.

It is crucial that the model reflect the fundamental processes of degradation as mechanistically as possible before follow-on modeling efforts attempting to expand the boundaries of the model by including factors associated with viewing a landfill as a cell such as climatic conditions are pursued. When these factors associated with the landfill cell are addressed in future efforts, the model can be fully applied in actual landfill management assessing landfill performance/impact over time and optimizing controllable parameters for biodegradation.

Final Assessment of the Thesis Effort

The biodegradation process of the landfill biochemical reactor is an extremely complex, dynamic system. In understanding this system, modeling the fundamental processes involved proves to be an invaluable tool. System dynamics modeling is an ideal approach to assessing such a changing system. By constructing the model and through model simulation, one learns how the system operates, what influences exist, how strong these influences are, and how essential the numerous interdependencies and feedback loops are to the functioning of the degradation process.

In contrast to other modeling approaches, system dynamics modeling focuses on what drives behavior for the *overall* defined system rather than concentrating on one particular influential aspect of the system. Instead of asking what drives the one particularly influential entity, system dynamics explores what drives the overall system. By laying the foundation for understanding and mechanistically modeling the fundamental processes of the landfill reactor, the model ultimately creates possibilities for

assessing landfill performance and assisting landfill managers in optimizing the management of their specific sites.

Appendix A: Model Assumptions

General Assumptions:

- Model Basis
  - Model is constructed on a mass basis. All relevant entities are assumed to be a generic mass unit or a mass unit/time flow or rate.
  - Derived stoichiometric equations denote all possible reaction possibilities for the degradation process of the landfill bioreactor system.
- Model Stocks
  - Initial organic waste is of the same composition ($C_{16}H_{34}O_{13}$).
  - No additional organic waste is placed into the system.
  - There are no substrates initially present in the system other than organic waste.
- Model Boundary
  - Model views landfill bioreactor system as a complete system. Management of the system (addition of moisture, etc.) is not addressed.
  - Only environmental entities directly responsible for the degradation process such as moisture content are included within the model's boundaries.
- Environmental Conditions
  - Environmental conditions are not influenced by factors external to the system such as climatic conditions.
  - The relationship between environmental conditions such as moisture content and each set of bacteria are modeled identically.
  - Saturated conditions support bacterial growth rates higher than normal bacterial growth rates given other model parameters provide optimal growth conditions.
  - Increased microbial activity cause increased temperatures not to exceed 60 deg C. Microbial activity is determined by bacterial growth rates.
- Bacteria
  - Each major category of bacteria represents all species of the category. Parameters such as cell yield for each category applies to all species.
  - Efficiency in substrate utilization and initial bacterial mass present for each set of bacteria generally decrease as degradation proceeds from aerobic degradation to methanogenesis (i.e. aerobic bacteria are more efficient and are present in greater mass initially than hydrolytic bacteria).
  - Methanogens will not utilize carbon dioxide and hydrogen as a substrate unless the combination exists in the appropriate ratio to support the stoichiometric equation defining the reaction responsible for the conversion of the substrate by methanogens.

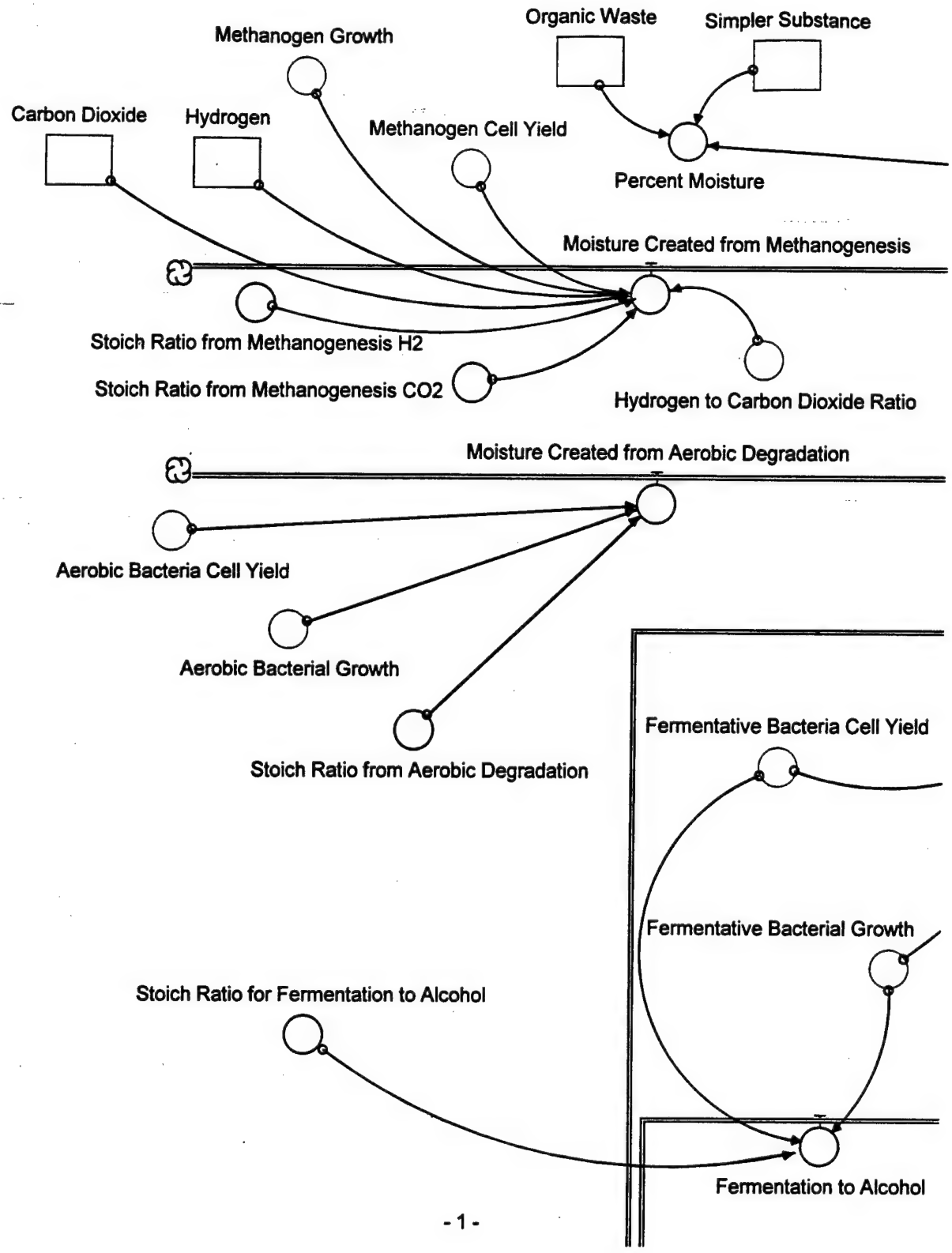
Detailed Assumptions:

Model Entity	Model Value	Assumption
Aerobe u_{max} (d^{-1})	1.0	The value is greater than all anaerobic bacteria due to known greater efficiency of aerobes and aerobic degradation compared to anaerobic bacteria and processes.
Aerobe Y	0.6	Highest Y to reflect greatest efficiency in converting substrate to energy.
Aerobe K (mg)	50	Again, the lowest K value of the bacterial groups involved demonstrates the efficiency of aerobes. Since no literature value was found for comparison, the value is chosen to reflect the efficiency concept. (Conceptually, they reach their maximum growth rate first.)
Hydrolytic Bacteria u_{max} (d^{-1})	0.5	Although a plausible value, it is artificially set at lower value than general assumption of efficiency dictates due to limitation of the model concerning substrate availability. No specific value for hydrolytic bacteria was found, but value based on efficiency concept and other anaerobic values found. See Structure Verification section.
Hydrolytic Bacteria Y	0.5	Y value between lowest anaerobic stage and aerobic stage to reflect efficiency of converting substrate to energy below that of aerobes but above other anaerobic species.
Hydrolytic Bacteria K (mg)	250	No specific value for hydrolytic bacteria was found, but value based on efficiency concept and other anaerobic values found. Highest K value of anaerobic bacteria to reflect general assumption regarding efficiency.
Fermentative Bacteria u_{max} (d^{-1})	0.6	Value reflects efficiency general assumption. Value greater than acetogen value. Rates vary depending on composition of substrate and experiment. Lower value used to emphasize field conditions vice optimal laboratory conditions.
Fermentative Bacteria Y	0.5	Y value between lowest anaerobic stage and aerobic stage to reflect efficiency of converting substrate to energy below that of aerobes but above other anaerobic species.

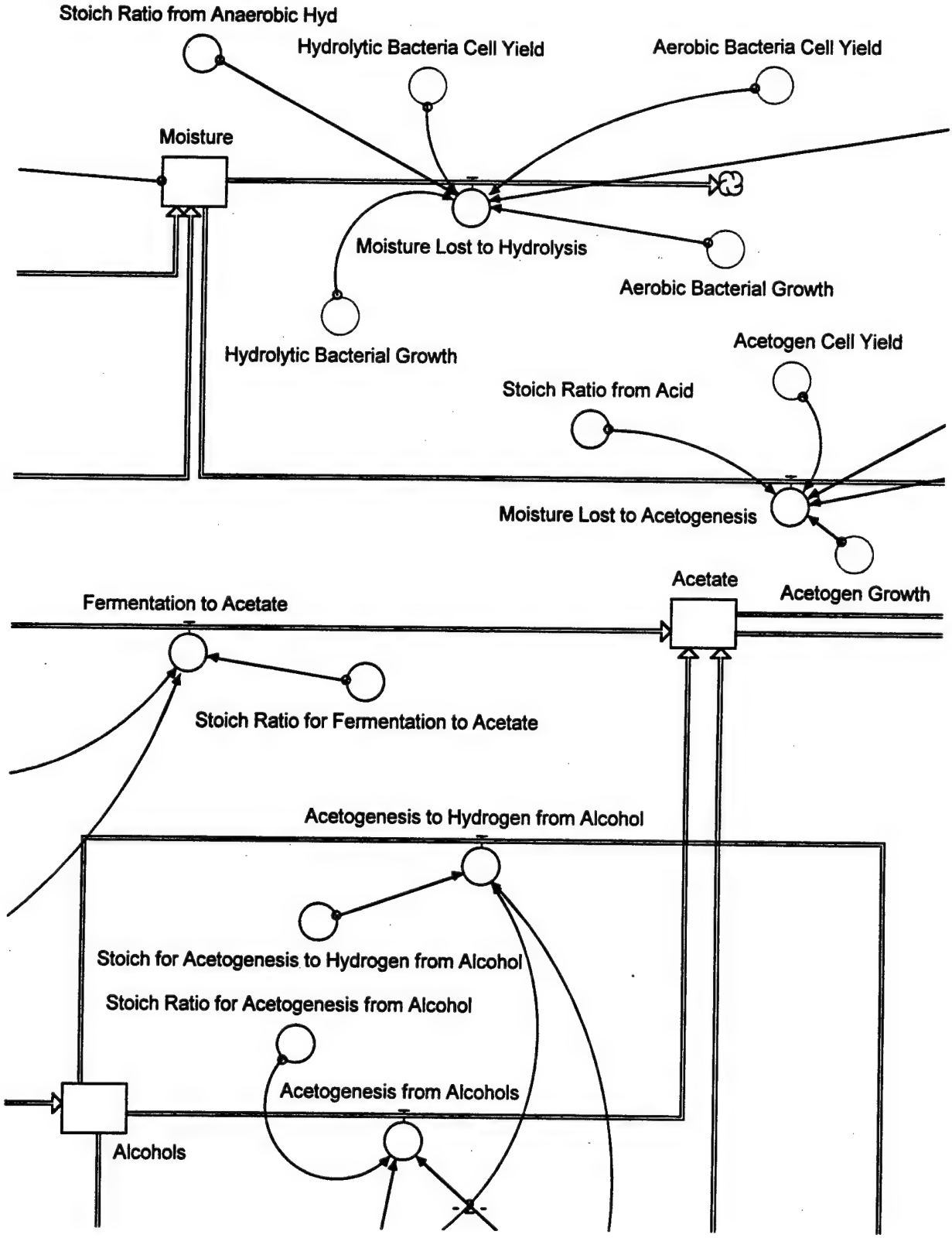
Fermentative Bacteria K (mg)	500	Value reflects efficiency general assumption. Value falls between hydrolytic bacteria and acetogen values. Model value from mass basis while literature value in concentration terms (mg/L).
Acetogen u_{max} (d^{-1})	0.55	Value reflects efficiency general assumption. Value falls between fermentative bacteria and methanogen values. Rates vary depending on composition of substrate and experiment. Lower value used to emphasize field conditions vice optimal laboratory conditions.
Acetogen Y	0.4	Y value reflects lowest efficiency of converting substrate to energy.
Acetogen K (mg)	750	Value reflects efficiency general assumption. Value falls between fermentative bacteria and methanogen values. Model value from mass basis while literature value in concentration terms (mg/L).
Methanogen u_{max} (d^{-1})	0.525	Value reflects efficiency general assumption. Value is lowest of all bacteria. Rates vary depending on composition of substrate and experiment. Lower value used to emphasize field conditions vice optimal laboratory conditions.
Methanogen Y	0.4	Y value reflects lowest efficiency of converting substrate to energy.
Methanogen K (mg)	1000	Value reflects efficiency general assumption. Value is highest of all bacteria. Model value from mass basis while literature value in concentration terms (mg/L).
Aerobe to Acetogen Decay Rates (d^{-1})	0.1	Based on fermentative bacterial rate. Only methanogen decay rates differed significantly in literature to warrant a separate numerical value.
Methanogen Decay Rate (d^{-1})	0.01	Only methanogen decay rates differed significantly to warrant a separate numerical value.
Initial Moisture Content	40%	See Environmental Parameter Section of Chapter 2.
Temperature	20-60	Represents rise of temperature from ambient as microbial activity increases until rise in temperature can become inhibitory. Initial temperature is 20 deg C.
Optimal pH for methanogens	6.4-7.4	Outside optimal range, pH becomes inhibitory to methanogens. Initial pH level is slightly above neutral (roughly 7.8).

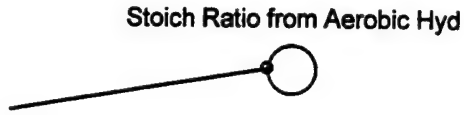
Appendix B: Model Structure

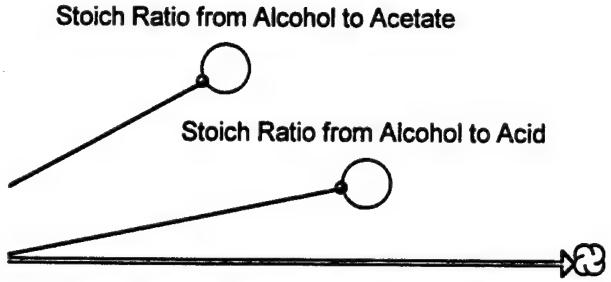
Due to the size of the model structure, the structure cannot be presented on a single sheet of paper. The following ten pages contain the structure. There are numerous breaks occurring in the presentation due to the necessity of utilizing more than one page to display the model and maintain readability.

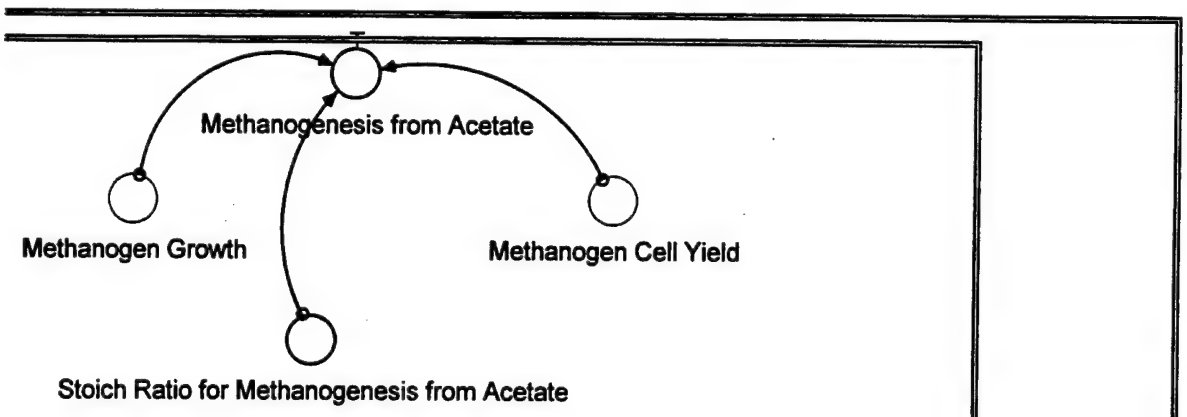

Organic Waste
Simpler Substance
Methanogen Growth
Carbon Dioxide
Hydrogen
Methanogen Cell Yield
Percent Moisture
Moisture Created from Methanogenesis
Stoich Ratio from Methanogenesis H2
Stoich Ratio from Methanogenesis CO2
Hydrogen to Carbon Dioxide Ratio
Moisture Created from Aerobic Degradation
Aerobic Bacteria Cell Yield
Aerobic Bacterial Growth
Stoich Ratio from Aerobic Degradation
Fermentative Bacteria Cell Yield
Fermentative Bacterial Growth
Stoich Ratio for Fermentation to Alcohol
Fermentation to Alcohol

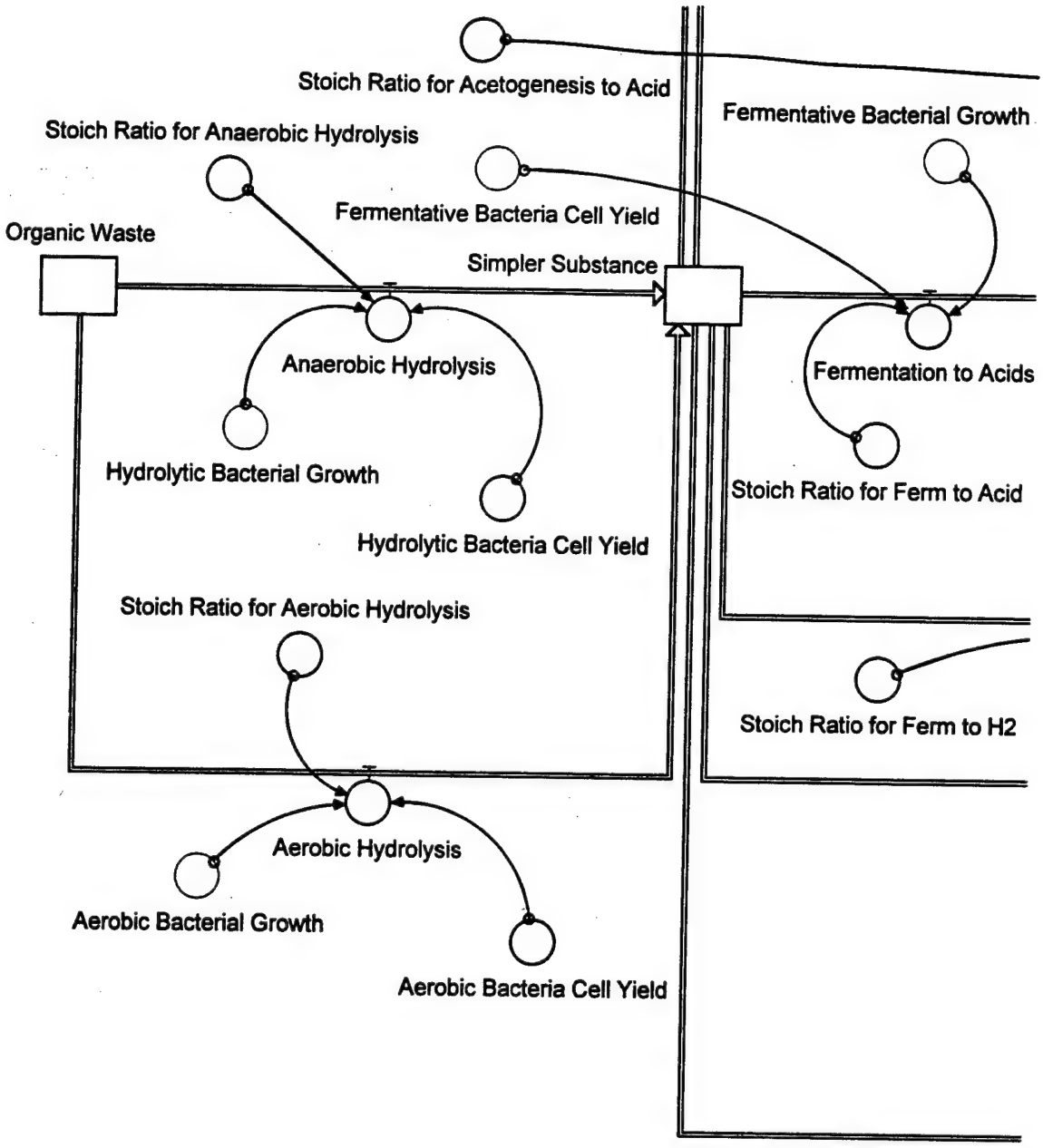
- 1 -

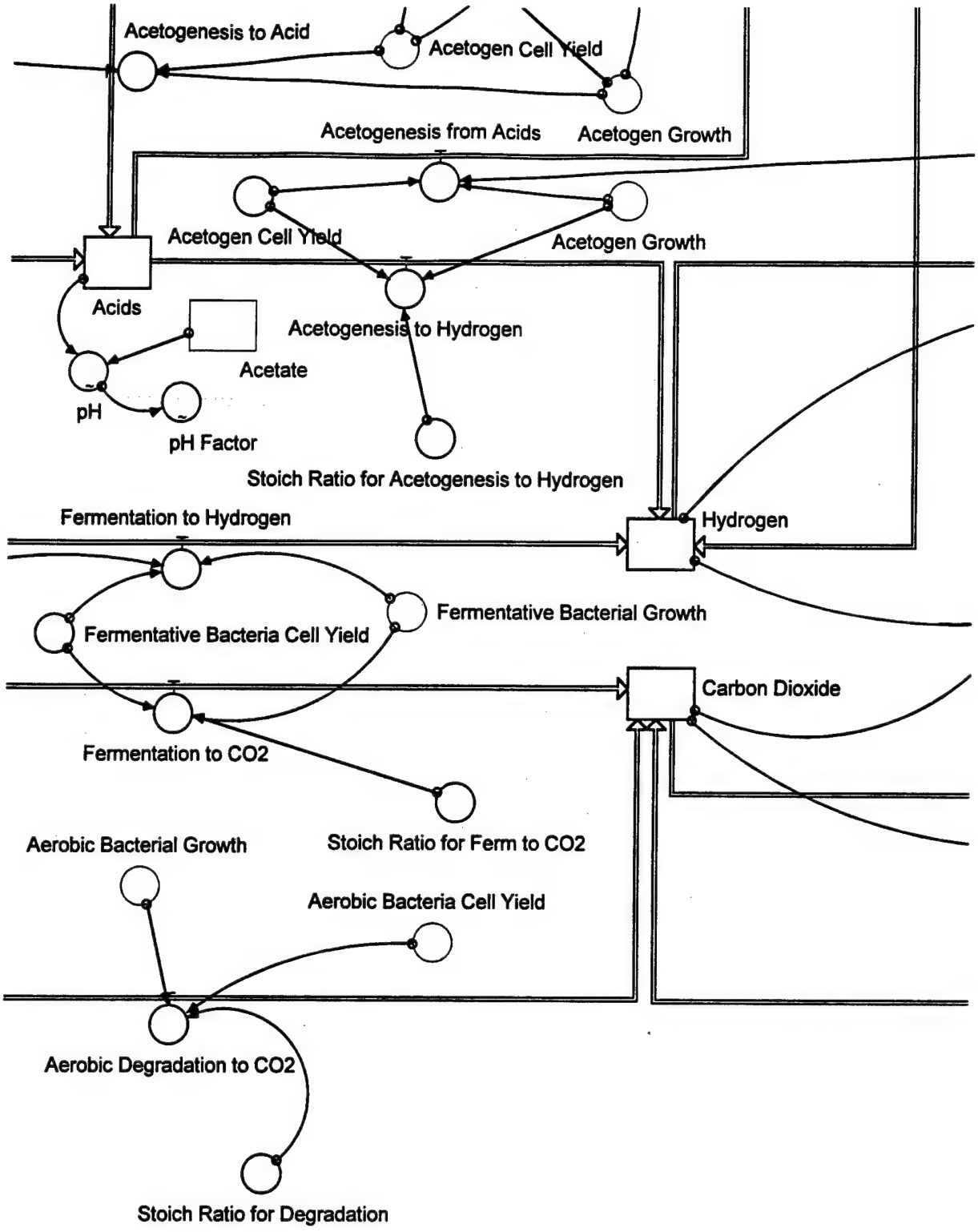

Stoich Ratio from Anaerobic Hyd
Hydrolytic Bacteria Cell Yield
Aerobic Bacteria Cell Yield
Moisture
Moisture Lost to Hydrolysis
Aerobic Bacterial Growth
Hydrolytic Bacterial Growth
Acetogen Cell Yield
Stoich Ratio from Acid
Moisture Lost to Acetogenesis
Acetate
Acetogen Growth
Fermentation to Acetate
Stoich Ratio for Fermentation to Acetate
Acetogenesis to Hydrogen from Alcohol
Stoich for Acetogenesis to Hydrogen from Alcohol
Stoich Ratio for Acetogenesis from Alcohol
Acetogenesis from Alcohols
Alcohols


Stoich Ratio from Aerobic Hyd

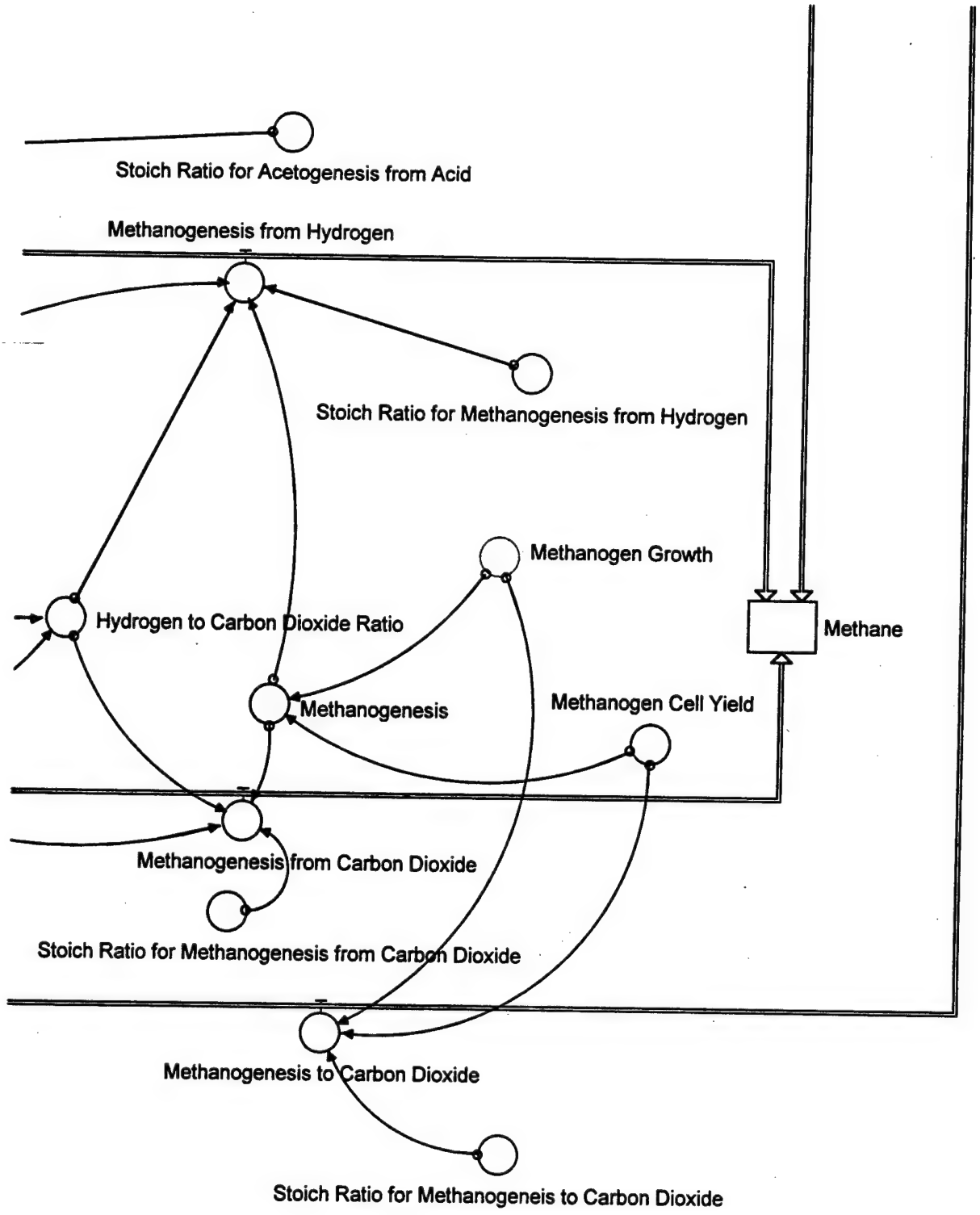

Stoich Ratio from Alcohol to Acetate
Stoich Ratio from Alcohol to Acid


Methanogenesis from Acetate
Methanogen Growth
Methanogen Cell Yield
Stoich Ratio for Methanogenesis from Acetate

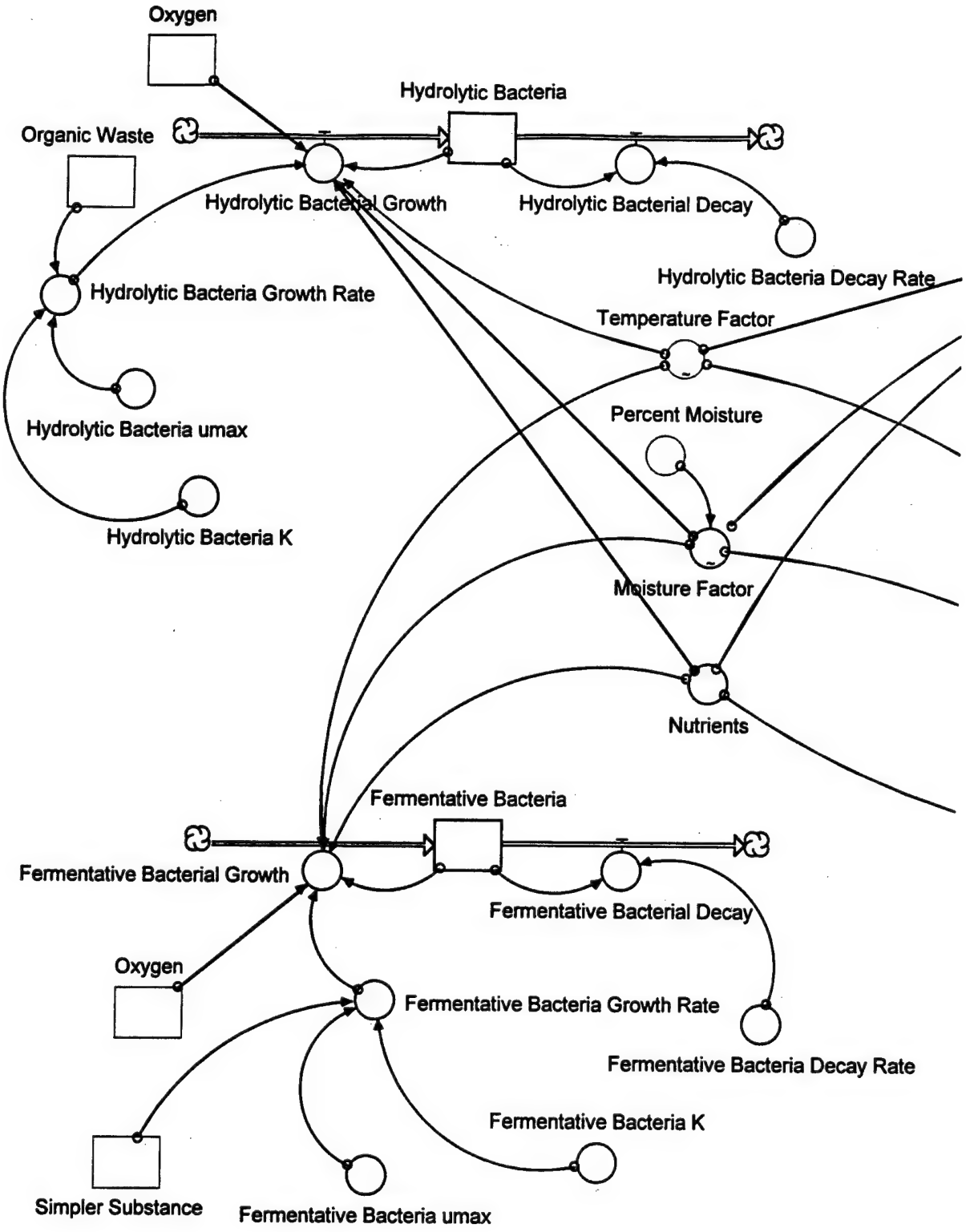

Stoich Ratio for Acetogenesis to Acid
Fermentative Bacterial Growth
Stoich Ratio for Anaerobic Hydrolysis
Fermentative Bacteria Cell Yield
Organic Waste
Simpler Substance
Anaerobic Hydrolysis
Fermentation to Acids
Hydrolytic Bacterial Growth
Stoich Ratio for Ferm to Acid
Hydrolytic Bacteria Cell Yield
Stoich Ratio for Aerobic Hydrolysis
Stoich Ratio for Ferm to H2
Aerobic Hydrolysis
Aerobic Bacterial Growth
Aerobic Bacteria Cell Yield


Acetogenesis to Acid
Acetogen Cell Yield
Acetogenesis from Acids
Acetogen Growth
Acetogen Cell Yield
Acetogen Growth
Acids
Acetogenesis to Hydrogen
Acetate
pH
pH Factor
Stoich Ratio for Acetogenesis to Hydrogen
Fermentation to Hydrogen
Hydrogen
Fermentative Bacterial Growth
Fermentative Bacteria Cell Yield
Carbon Dioxide
Fermentation to CO2
Stoich Ratio for Ferm to CO2
Aerobic Bacterial Growth
Aerobic Bacteria Cell Yield
Aerobic Degradation to CO2
Stoich Ratio for Degradation

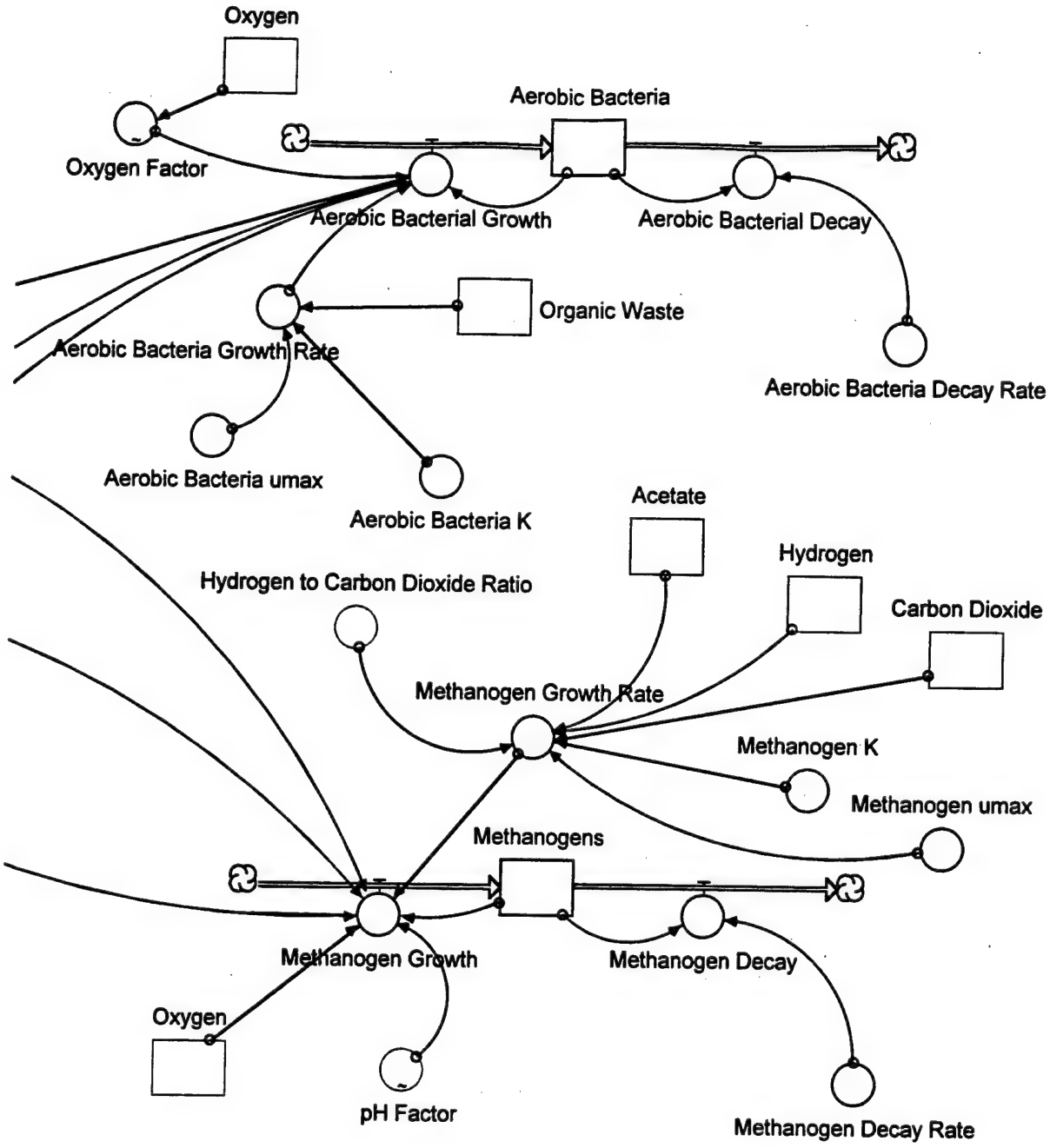
- 5 -

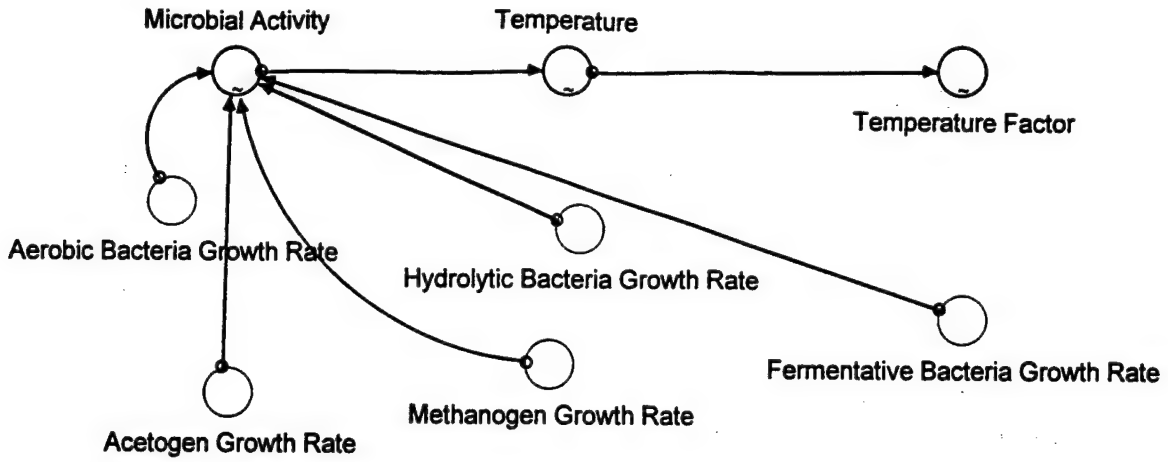

Stoich Ratio for Acetogenesis from Acid
Methanogenesis from Hydrogen
Stoich Ratio for Methanogenesis from Hydrogen
Methanogen Growth
Hydrogen to Carbon Dioxide Ratio
Methane
Methanogenesis
Methanogen Cell Yield
Methanogenesis from Carbon Dioxide
Stoich Ratio for Methanogenesis from Carbon Dioxide
Methanogenesis to Carbon Dioxide
Stoich Ratio for Methanogeneis to Carbon Dioxide

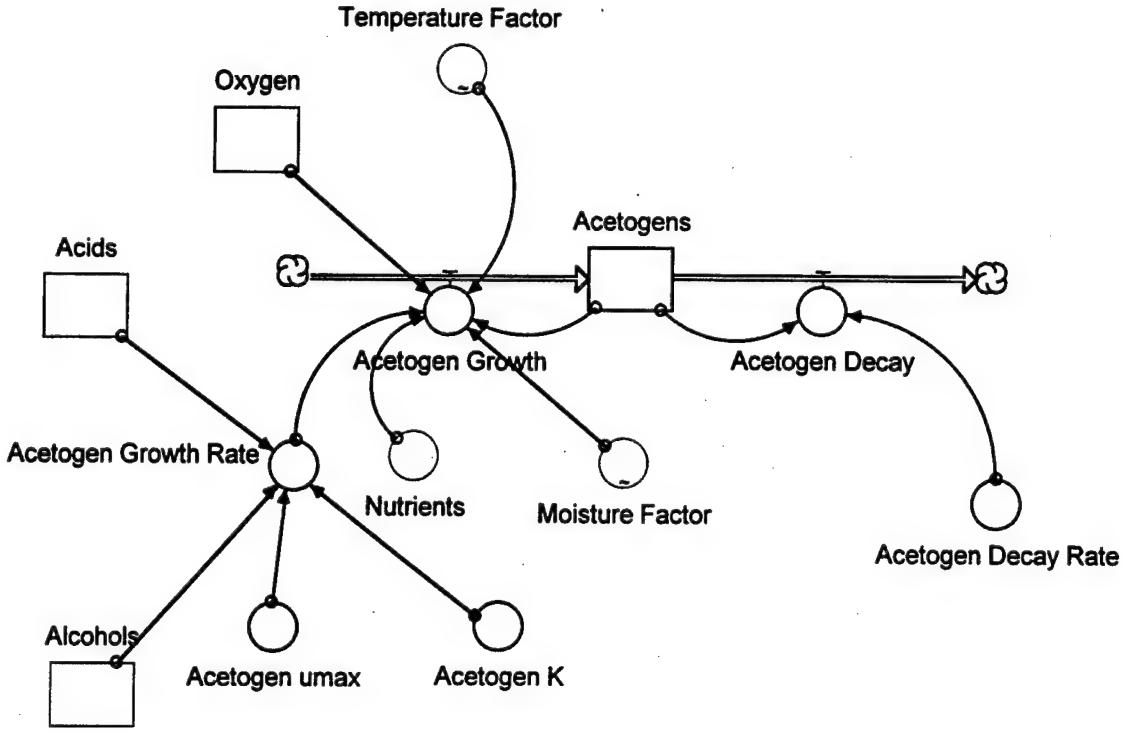
- 6 -

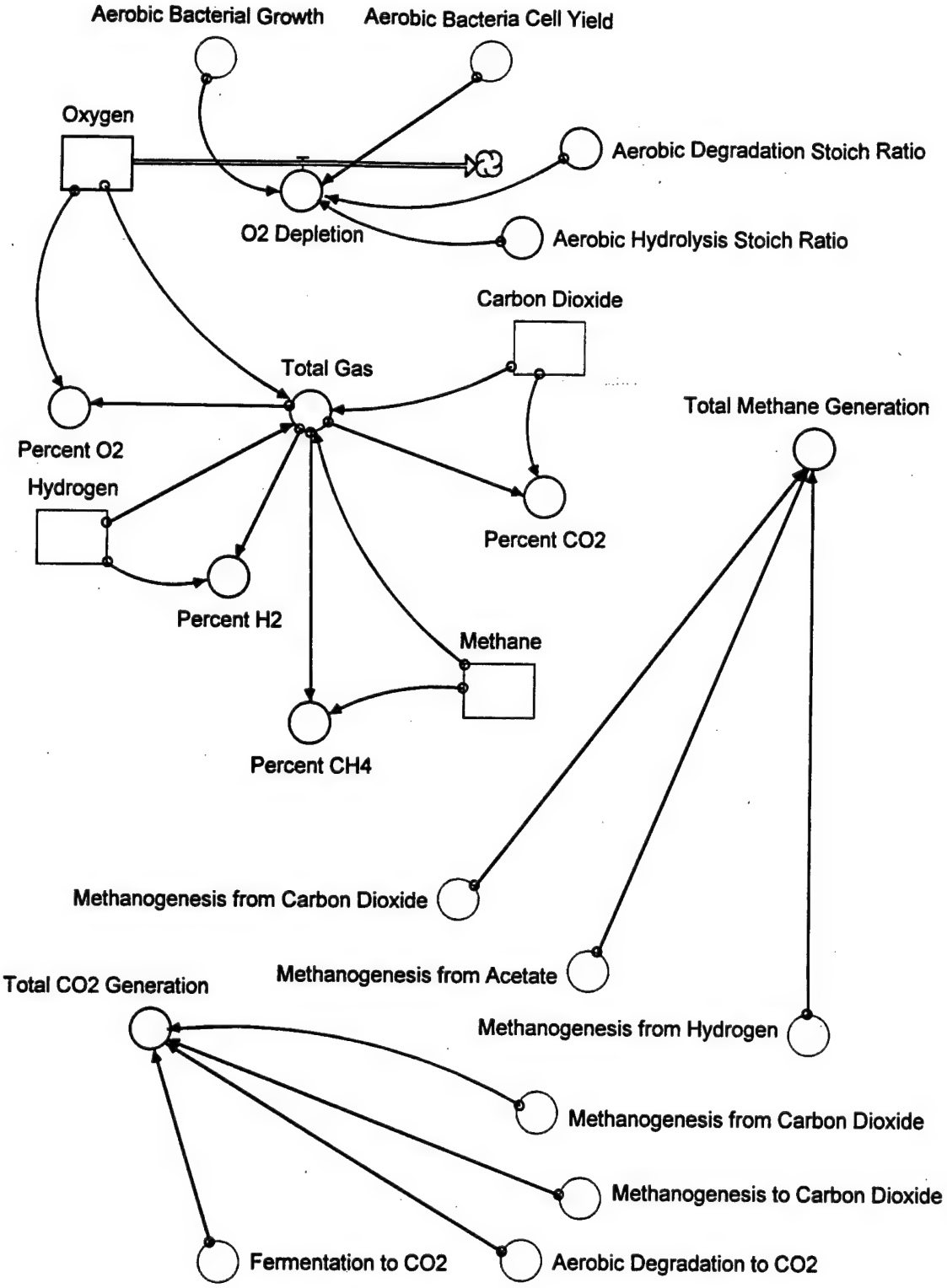

Oxygen
Hydrolytic Bacteria
Organic Waste
Hydrolytic Bacterial Growth
Hydrolytic Bacterial Decay
Hydrolytic Bacteria Decay Rate
Hydrolytic Bacteria Growth Rate
Temperature Factor
Percent Moisture
Hydrolytic Bacteria umax
Hydrolytic Bacteria K
Moisture Factor
Nutrients
Fermentative Bacteria
Fermentative Bacterial Growth
Fermentative Bacterial Decay
Oxygen
Fermentative Bacteria Growth Rate
Fermentative Bacteria Decay Rate
Fermentative Bacteria K
Simpler Substance
Fermentative Bacteria umax

- 7 -


Oxygen
Aerobic Bacteria
Oxygen Factor
Aerobic Bacterial Growth
Aerobic Bacterial Decay
Organic Waste
Aerobic Bacteria Growth Rate
Aerobic Bacteria Decay Rate
Aerobic Bacteria umax
Aerobic Bacteria K
Acetate
Hydrogen
Hydrogen to Carbon Dioxide Ratio
Carbon Dioxide
Methanogen Growth Rate
Methanogen K
Methanogen umax
Methanogens
Methanogen Growth
Methanogen Decay
Oxygen
pH Factor
Methanogen Decay Rate


Microbial Activity
Temperature
Temperature Factor
Aerobic Bacteria Growth Rate
Hydrolytic Bacteria Growth Rate
Fermentative Bacteria Growth Rate
Acetogen Growth Rate
Methanogen Growth Rate


Temperature Factor
Oxygen
Acetogens
Acids
Acetogen Growth
Acetogen Decay
Acetogen Growth Rate
Nutrients
Moisture Factor
Acetogen Decay Rate
Alcohols
Acetogen umax
Acetogen K


Aerobic Bacterial Growth
Aerobic Bacteria Cell Yield
Oxygen
Aerobic Degradation Stoich Ratio
O2 Depletion
Aerobic Hydrolysis Stoich Ratio
Carbon Dioxide
Total Gas
Total Methane Generation
Percent O2
Hydrogen
Percent CO2
Percent H2
Methane
Percent CH4
Methanogenesis from Carbon Dioxide
Total CO2 Generation
Methanogenesis from Acetate
Methanogenesis from Hydrogen
Methanogenesis from Carbon Dioxide
Methanogenesis to Carbon Dioxide
Fermentation to CO2
Aerobic Degradation to CO2

Appendix C: Model Equations

Due to the number of the model equations denoting the various processes of the landfill bioreactor system, the equations cannot be presented on a single sheet of paper. The following seven pages contain the equations.

Acetate(t) = Acetate(t - dt) + (Acetogenesis_from_Acids + Acetogenesis_from_Alcohols + Fermentation_to_Acetate - Methanogenesis_from_Acetate - Methanogenesis_to_Carbon_Dioxide) * dt
INIT Acetate = 0

INFLOWS:
- Acetogenesis_from_Acids = Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_Ratio_for_Acetogenesis_from_Acid
- Acetogenesis_from_Alcohols = Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_Ratio_for_Acetogenesis_from_Alcohol
- Fermentation_to_Acetate = Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Fermentation_to_Acetate

OUTFLOWS:
- Methanogenesis_from_Acetate = Methanogen_Growth*(1/Methanogen_Cell_Yield)*Stoich_Ratio_for_Methanogenesis_from_Acetate
- Methanogenesis_to_Carbon_Dioxide = Methanogen_Growth*(1/Methanogen_Cell_Yield)*Stoich_Ratio_for_Methanogeneis_to_Carbon_Dioxide

Acetogens(t) = Acetogens(t - dt) + (Acetogen_Growth - Acetogen_Decay) * dt
INIT Acetogens = 100

INFLOWS:
- Acetogen_Growth = IF(Oxygen=0)AND(Nutrients=1)THEN(Acetogens*(Acetogen_Growth_Rate*Moisture_Factor*Temperature_Factor))ELSE(0)

OUTFLOWS:
- Acetogen_Decay = Acetogens*Acetogen_Decay_Rate

Acids(t) = Acids(t - dt) + (Fermentation_to_Acids + Acetogenesis_to_Acid - Acetogenesis_to_Hydrogen - Acetogenesis_from_Acids) * dt
INIT Acids = 0

INFLOWS:
- Fermentation_to_Acids = Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Ferm_to_Acid
- Acetogenesis_to_Acid = Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_Ratio_for_Acetogenesis_to_Acid

OUTFLOWS:
- Acetogenesis_to_Hydrogen = Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_Ratio_for_Acetogenesis_to_Hydrogen
- Acetogenesis_from_Acids = Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_Ratio_for_Acetogenesis_from_Acid

Aerobic_Bacteria(t) = Aerobic_Bacteria(t - dt) + (Aerobic_Bacterial_Growth - Aerobic_Bacterial_Decay) * dt
INIT Aerobic_Bacteria = 10000

INFLOWS:

Aerobic_Bacterial_Growth =
IF(Nutrients=1)THEN(Aerobic_Bacteria*(Aerobic_Bacteria_Growth_Rate*Moisture_Factor*Temperature_Factor*Oxygen_Factor))ELSE(0)

OUTFLOWS:

Aerobic_Bacterial_Decay = Aerobic_Bacteria*Aerobic_Bacteria_Decay_Rate

Alcohols(t) = Alcohols(t - dt) + (Fermentation_to_Alcohol - Acetogenesis_to_Acid - Acetogenesis_from_Alcohols - Acetogenesis_to_Hydrogen_from_Alcohol) * dt

INIT Alcohols = 0

INFLOWS:

Fermentation_to_Alcohol =
Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Fermentation_to_Alcohol

OUTFLOWS:

Acetogenesis_to_Acid =
Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_Ratio_for_Acetogenesis_to_Acid

Acetogenesis_from_Alcohols =
Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_Ratio_for_Acetogenesis_from_Alcohol

Acetogenesis_to_Hydrogen_from_Alcohol =
Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_for_Acetogenesis_to_Hydrogen_from_Alcohol

Carbon_Dioxide(t) = Carbon_Dioxide(t - dt) + (Fermentation_to_CO2 + Aerobic_Degradation_to_CO2 + Methanogenesis_to_Carbon_Dioxide - Methanogenesis_from_Carbon_Dioxide) * dt

INIT Carbon_Dioxide = 0

INFLOWS:

Fermentation_to_CO2 =
Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Ferm_to_CO2

Aerobic_Degradation_to_CO2 =
Aerobic_Bacterial_Growth*(1/Aerobic_Bacteria_Cell_Yield)*Stoich_Ratio_for_Degradation

Methanogenesis_to_Carbon_Dioxide =
Methanogen_Growth*(1/Methanogen_Cell_Yield)*Stoich_Ratio_for_Methanogeneis_to_Carbon_Dioxide

OUTFLOWS:

Methanogenesis_from_Carbon_Dioxide =
IF((Hydrogen_to_Carbon_Dioxide_Ratio<.18)AND(Carbon_Dioxide>=44))THEN(Methanogenesis*Stoich_Ratio_for_Methanogenesis_from_Carbon_Dioxide)ELSE(0)

Fermentative_Bacteria(t) = Fermentative_Bacteria(t - dt) + (Fermentative_Bacterial_Growth - Fermentative_Bacterial_Decay) * dt

INIT Fermentative_Bacteria = 1000

INFLOWS:

Fermentative_Bacterial_Growth =
IF(Oxygen=0)AND(Nutrients=1)THEN(Fermentative_Bacteria*(Fermentative_Bacteria_Growth_Rate*Moisture_Factor*Temperature_Factor))ELSE(0)

OUTFLOWS:

Fermentative_Bacterial_Decay = Fermentative_Bacteria*Fermentative_Bacteria_Decay_Rate

Hydrogen(t) = Hydrogen(t - dt) + (Fermentation_to_Hydrogen + Acetogenesis_to_Hydrogen + Acetogenesis_to_Hydrogen_from_Alcohol - Methanogenesis_from_Hydrogen) * dt
INIT Hydrogen = 0
INFLOWS:
Fermentation_to_Hydrogen = Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Ferm_to_H2
Acetogenesis_to_Hydrogen = Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_Ratio_for_Acetogenesis_to_Hydrogen
Acetogenesis_to_Hydrogen_from_Alcohol = Acetogen_Growth*(1/Acetogen_Cell_Yield)*Stoich_for_Acetogenesis_to_Hydrogen_from_Alcohol
OUTFLOWS:
Methanogenesis_from_Hydrogen = IF((Hydrogen_to_Carbon_Dioxide_Ratio<.18)AND(Hydrogen>=8))THEN(Methanogenesis*Stoich_Ratio_for_Methanogenesis_from_Hydrogen)ELSE(0)

Hydrolytic_Bacteria(t) = Hydrolytic_Bacteria(t - dt) + (Hydrolytic_Bacterial_Growth - Hydrolytic_Bacterial_Decay) * dt
INIT Hydrolytic_Bacteria = 1000
INFLOWS:
Hydrolytic_Bacterial_Growth = IF(Oxygen=0)AND(Nutrients=1)THEN(Hydrolytic_Bacteria*(Hydrolytic_Bacteria_Growth_Rate*Moisture_Factor*Temperature_Factor))ELSE(0)
OUTFLOWS:
Hydrolytic_Bacterial_Decay = Hydrolytic_Bacteria*Hydrolytic_Bacteria_Decay_Rate

Methane(t) = Methane(t - dt) + (Methanogenesis_from_Carbon_Dioxide + Methanogenesis_from_Hydrogen + Methanogenesis_from_Acetate) * dt
INIT Methane = 0
INFLOWS:
Methanogenesis_from_Carbon_Dioxide = IF((Hydrogen_to_Carbon_Dioxide_Ratio<.18)AND(Carbon_Dioxide>=44))THEN(Methanogenesis*Stoich_Ratio_for_Methanogenesis_from_Carbon_Dioxide)ELSE(0)
Methanogenesis_from_Hydrogen = IF((Hydrogen_to_Carbon_Dioxide_Ratio<.18)AND(Hydrogen>=8))THEN(Methanogenesis*Stoich_Ratio_for_Methanogenesis_from_Hydrogen)ELSE(0)
Methanogenesis_from_Acetate = Methanogen_Growth*(1/Methanogen_Cell_Yield)*Stoich_Ratio_for_Methanogenesis_from_Acetate

Methanogens(t) = Methanogens(t - dt) + (Methanogen_Growth - Methanogen_Decay) * dt
INIT Methanogens = 100
INFLOWS:
Methanogen_Growth = IF(Oxygen=0)AND(Nutrients=1)THEN(Methanogens*(Methanogen_Growth_Rate*Moisture_Factor*Temperature_Factor*pH_Factor))ELSE(0)

OUTFLOWS:

Methanogen_Decay = Methanogens*Methanogen_Decay_Rate

Moisture(t) = Moisture(t - dt) + (Moisture_Created_from_Aerobic_Degradation + Moisture_Created_from_Methanogenesis - Moisture_Lost_to_Hydrolysis - Moisture_Lost_to_Acetogenesis) * dt

INIT Moisture = 400000000000000000000000000000000000000000000000

INFLOWS:

Moisture_Created_from_Aerobic_Degradation = Aerobic_Bacterial_Growth*(1/Aerobic_Bacteria_Cell_Yield)*Stoich_Ratio_from_Aerobic_Degradation

Moisture_Created_from_Methanogenesis = IF(Hydrogen_to_Carbon_Dioxide_Ratio<.18)AND(Hydrogen>=8)AND(Carbon_Dioxide>=44)THEN((Methanogen_Growth*(1/Methanogen_Cell_Yield)*Stoich_Ratio_from_Methanogenesis_H2)+(Methanogen_Growth*(1/Methanogen_Cell_Yield)*Stoich_Ratio_from_Methanogenesis_CO2))ELSE(0)

OUTFLOWS:

Moisture_Lost_to_Hydrolysis = (Aerobic_Bacterial_Growth*(1/Aerobic_Bacteria_Cell_Yield)*Stoich_Ratio_from_Aerobic_Hyd)+(Hydrolytic_Bacterial_Growth*(1/Hydrolytic_Bacteria_Cell_Yield)*Stoich_Ratio_from_Anaerobic_Hyd)

Moisture_Lost_to_Acetogenesis = (Stoich_Ratio_from_Acid*Acetogen_Growth*(1/Acetogen_Cell_Yield))+(Stoich_Ratio_from_Acid*Acetogen_Growth*(1/Acetogen_Cell_Yield))+(Stoich_Ratio_from_Alcohol_to_Acetate*Acetogen_Growth*(1/Acetogen_Cell_Yield))+(Stoich_Ratio_from_Alcohol_to_Acid*Acetogen_Growth*(1/Acetogen_Cell_Yield))

Organic_Waste(t) = Organic_Waste(t - dt) + (- Aerobic_Hydrolysis - Anaerobic_Hydrolysis) * dt

INIT Organic_Waste = 1000000000000000000000000000000000000000000000000

OUTFLOWS:

Aerobic_Hydrolysis = Aerobic_Bacterial_Growth*(1/Aerobic_Bacteria_Cell_Yield)*Stoich_Ratio_for_Aerobic_Hydrolysis

Anaerobic_Hydrolysis = Hydrolytic_Bacterial_Growth*(1/Hydrolytic_Bacteria_Cell_Yield)*Stoich_Ratio_for_Anaerobic_Hydrolysis

Oxygen(t) = Oxygen(t - dt) + (- O2_Depletion) * dt

INIT Oxygen = 100000000

OUTFLOWS:

O2_Depletion = (Aerobic_Bacterial_Growth*(1/Aerobic_Bacteria_Cell_Yield)*Aerobic_Hydrolysis_Stoich_Ratio)+(Aerobic_Bacterial_Growth*(1/Aerobic_Bacteria_Cell_Yield)*Aerobic_Degradation_Stoich_Ratio)

Simpler_Substance(t) = Simpler_Substance(t - dt) + (Aerobic_Hydrolysis + Anaerobic_Hydrolysis - Fermentation_to_CO2 - Aerobic_Degradation_to_CO2 - Fermentation_to_Hydrogen - Fermentation_to_Acids - Fermentation_to_Alcohol - Fermentation_to_Acetate) * dt

INIT Simpler_Substance = 0

INFLOWS:

- Aerobic_Hydrolysis = Aerobic_Bacterial_Growth*(1/Aerobic_Bacteria_Cell_Yield)*Stoich_Ratio_for_Aerobic_Hydrolysis
- Anaerobic_Hydrolysis = Hydrolytic_Bacterial_Growth*(1/Hydrolytic_Bacteria_Cell_Yield)*Stoich_Ratio_for_Anaerobic_Hydrolysis

OUTFLOWS:

- Fermentation_to_CO2 = Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Ferm_to_CO2
- Aerobic_Degradation_to_CO2 = Aerobic_Bacterial_Growth*(1/Aerobic_Bacteria_Cell_Yield)*Stoich_Ratio_for_Degradation
- Fermentation_to_Hydrogen = Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Ferm_to_H2
- Fermentation_to_Acids = Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Ferm_to_Acid
- Fermentation_to_Alcohol = Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Fermentation_to_Alcohol
- Fermentation_to_Acetate = Fermentative_Bacterial_Growth*(1/Fermentative_Bacteria_Cell_Yield)*Stoich_Ratio_for_Fermentation_to_Acetate

- Acetogen_Cell_Yield = .4
- Acetogen_Decay_Rate = .1
- Acetogen_Growth_Rate = MAX(Acetogen_umax*((Acids)/(Acetogen_K+Acids)),Acetogen_umax*((Alcohols)/(Acetogen_K+Alcohols)))
- Acetogen_K = 750
- Acetogen_umax = .55
- Aerobic_Bacteria_Cell_Yield = .6
- Aerobic_Bacteria_Decay_Rate = .1
- Aerobic_Bacteria_Growth_Rate = ((Aerobic_Bacteria_umax*Organic_Waste)/(Aerobic_Bacteria_K+Organic_Waste))
- Aerobic_Bacteria_K = 50
- Aerobic_Bacteria_umax = 1
- Aerobic_Degradation_Stoich_Ratio = 1.2
- Aerobic_Hydrolysis_Stoich_Ratio = 9.2
- Fermentative_Bacteria_Cell_Yield = .5
- Fermentative_Bacteria_Decay_Rate = .1
- Fermentative_Bacteria_Growth_Rate = ((Fermentative_Bacteria_umax*Simpler_Substance)/(Fermentative_Bacteria_K+Simpler_Substance))

- Fermentative_Bacteria_K = 500
- Fermentative_Bacteria_umax = .6
- Hydrogen_to_Carbon_Dioxide_Ratio = Hydrogen/Carbon_Dioxide
- Hydrolytic_Bacteria_Cell_Yield = .5
- Hydrolytic_Bacteria_Decay_Rate = .1
- Hydrolytic_Bacteria_Growth_Rate = ((Hydrolytic_Bacteria_umax*Organic_Waste)/(Hydrolytic_Bacteria_K+Organic_Waste))
- Hydrolytic_Bacteria_K = 250
- Hydrolytic_Bacteria_umax = .5
- Methanogenesis = Methanogen_Growth*(1/Methanogen_Cell_Yield)
- Methanogen_Cell_Yield = .4
- Methanogen_Decay_Rate = .01
- Methanogen_Growth_Rate = IF((Hydrogen_to_Carbon_Dioxide_Ratio<.18)AND(Hydrogen>0)AND(Acetate>0))THEN(MAX((Methanogen_umax*Carbon_Dioxide*Hydrogen)/((Methanogen_K+Carbon_Dioxide)*(Methanogen_K+Hydrogen)),((Methanogen_umax*Acetate)/(Methanogen_K+Acetate))))ELSE((Methanogen_umax*Acetate)/(Methanogen_K+Acetate))
- Methanogen_K = 1000
- Methanogen_umax = .525
- Nutrients = 1
- Percent_CH4 = Methane/Total_Gas
- Percent_CO2 = Carbon_Dioxide/Total_Gas
- Percent_H2 = Hydrogen/Total_Gas
- Percent_Moisture = Moisture/(Organic_Waste+Simpler_Substance)
- Percent_O2 = Oxygen/Total_Gas
- Stoich_for_Acetogenesis_to_Hydrogen_from_Alcohol = .09
- Stoich_Ratio_for_Acetogenesis_from_Acid = 1.2
- Stoich_Ratio_for_Acetogenesis_from_Alcohol = 1.3
- Stoich_Ratio_for_Acetogenesis_to_Acid = 1.2
- Stoich_Ratio_for_Acetogenesis_to_Hydrogen = .03
- Stoich_Ratio_for_Aerobic_Hydrolysis = 1
- Stoich_Ratio_for_Anaerobic_Hydrolysis = 1
- Stoich_Ratio_for_Degradation = 1.5
- Stoich_Ratio_for_Fermentation_to_Acetate = .3
- Stoich_Ratio_for_Fermentation_to_Alcohol = .2
- Stoich_Ratio_for_Ferm_to_Acid = .3
- Stoich_Ratio_for_Ferm_to_CO2 = .19
- Stoich_Ratio_for_Ferm_to_H2 = .009
- Stoich_Ratio_for_Methanogeneis_to_Carbon_Dioxide = .7
- Stoich_Ratio_for_Methanogenesis_from_Acetate = .3
- Stoich_Ratio_for_Methanogenesis_from_Carbon_Dioxide = .4
- Stoich_Ratio_for_Methanogenesis_from_Hydrogen = 2
- Stoich_Ratio_from_Acid = .2
- Stoich_Ratio_from_Aerobic_Degradation = .7
- Stoich_Ratio_from_Aerobic_Hyd = .1

- Stoich_Ratio_from_Alcohol_to_Acetate = .4
- Stoich_Ratio_from_Alcohol_to_Acid = .3
- Stoich_Ratio_from_Anaerobic_Hyd = .04
- Stoich_Ratio_from_Methanogenesis_CO2 = .8
- Stoich_Ratio_from_Methanogenesis_H2 = 4.5
- Total_CO2_Generation = (Aerobic_Degradation_to_CO2+Fermentation_to_CO2+Methanogenesis_to_Carbon_Dioxide)-Methanogenesis_from_Carbon_Dioxide
- Total_Gas = Oxygen+Carbon_Dioxide+Hydrogen+Methane
- Total_Methane_Generation = Methanogenesis_from_Acetate+Methanogenesis_from_Carbon_Dioxide+Methanogenesis_from_Hydrogen
- Microbial_Activity = GRAPH(Aerobic_Bacteria_Growth_Rate+Acetogen_Growth_Rate+Fermentative_Bacteria_Growth_Rate+Hydrolytic_Bacteria_Growth_Rate+Methanogen_Growth_Rate)
  (0.00, 0.00), (0.35, 0.05), (0.7, 0.0875), (1.05, 0.106), (1.40, 0.156), (1.75, 0.206), (2.10, 0.3), (2.45, 0.4), (2.80, 0.575), (3.15, 0.775), (3.50, 1.25)
- Moisture_Factor = GRAPH(Percent_Moisture)
  (0.00, 0.00), (0.1, 0.45), (0.2, 0.66), (0.3, 0.833), (0.4, 1.00), (0.5, 1.19), (0.6, 1.31), (0.7, 1.38), (0.8, 1.43), (0.9, 1.47), (1, 1.50)
- Oxygen_Factor = GRAPH(Oxygen)
  (0.00, 0.005), (10.0, 0.085), (20.0, 0.205), (30.0, 0.295), (40.0, 0.41), (50.0, 0.495), (60.0, 0.615), (70.0, 0.705), (80.0, 0.795), (90.0, 0.905), (100, 0.995)
- pH = GRAPH(Acids+Acetate)
  (0.00, 7.80), (1e+011, 7.70), (2e+011, 7.60), (3e+011, 7.50), (4e+011, 7.40), (5e+011, 7.20), (6e+011, 7.00), (7e+011, 6.80), (8e+011, 6.60), (9e+011, 6.50), (1e+012, 6.45)
- pH_Factor = GRAPH(pH)
  (4.00, 0.00), (4.40, 0.00), (4.80, 0.00), (5.20, 0.00), (5.60, 0.00), (6.00, 0.1), (6.40, 1.00), (6.80, 1.00), (7.20, 1.00), (7.60, 0.96), (8.00, 0.00)
- Temperature = GRAPH(Microbial_Activity)
  (0.00, 20.0), (0.125, 32.6), (0.25, 40.4), (0.375, 43.8), (0.5, 46.4), (0.625, 49.0), (0.75, 51.4), (0.875, 53.2), (1.00, 55.6), (1.13, 57.6), (1.25, 60.0)
- Temperature_Factor = GRAPH(Temperature)
  (0.00, 0.00), (6.00, 0.025), (12.0, 0.08), (18.0, 0.24), (24.0, 0.61), (30.0, 0.89), (36.0, 1.00), (42.0, 1.00), (48.0, 1.00), (54.0, 0.905), (60.0, 0.005)

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13. ABSTRACT *(Maximum 200 words)*

Greater demands on landfill capacity, stricter regulations intended to minimize landfill environmental impacts, and the economic potential associated with landfill operations have shifted the emphasis of landfill disposal toward methods concerned with the long-term performance and capacity of landfills. Two opposing philosophies have emerged in constructing and managing landfills: the "dry-tomb" and the "wet-cell." The key to managing a landfill from the wet-cell viewpoint is first understanding the biodegradation processes occurring within the landfill.

This thesis attempts to determine the fundamental processes responsible for the degradation of solid waste by employing a system dynamics approach. A system dynamics model is constructed that reproduces behavior of the landfill biochemical reactor system by identifying the biodegradation processes driving basic system behavior. The model utilizes landfill gas production as the measure of landfill behavior over time. The resultant model and model simulations suggest that biodegradation is an extremely complex and dynamic process with numerous interrelationships and influences existing between the entities of the landfill system. With further development, the model may be applied by landfill managers concerned with assessing landfill performance/impact over time and optimizing controllable parameters for biodegradation.

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